

8th WEEK OF THE YOUNG RESEARCHER

CHEMICAL ENERGY STORAGE AND CONVERSION

German-Russian Institute
of Advanced Technologies (GRIAT)
Kazan National Research Technical University
named after A. N. Tupolev – KAI
Kazan, September 10–13, 2018

REPORT



IMPRESSUM

Volume of the Conference "The Eighth German-Russian Week of the Young Researcher"

Kazan, September 10–13, 2018

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WELCOME TO THE EIGHTH GERMAN-RUSSIAN WEEK OF THE YOUNG RESEARCHER!

Dear colleagues from Russia and Germany,

We are very delighted to welcome you to our Eighth Week of the Young Researcher! When we convened the “German-Russian Year of Science“, eight years ago, the idea was born to invite young researchers from both countries to come together to discuss current topics of mutual interest. The success of the first week in Kazan encouraged us to turn it into an annual event. The following years we met in Ekaterinburg (2012), Novosibirsk (2013), St. Petersburg (2014) and Moscow (2015, 2016, and 2017). The main goal of these meetings is to foster collaboration among young scientists and researchers who will be setting the agenda of scientific cooperation between Russia and Germany in the near future.

Research organizations and institutions of higher education of both our countries will be presenting their funding programmes and describing the platforms that they can offer to both Russian and German PhD students as well as PostDoctoral researchers. The overarching principle behind these presentations is to facilitate collaboration and to broaden research networks. The brochure illustrates how young and experienced scientists can work across borders with local authorities, asso-

ciations and industry in order to develop new approaches to global challenges.

This time we took an interdisciplinary approach and discussed particular topics of interest for chemical energy storage and conversion. Special emphasis was given to the challenges for improved materials and processes and their potential impact on existing and future applications and innovation. The organizers strove for a good mix of participants at different career stages and different fields of expertise that include contributions from Materials Chemistry, Physical Chemistry, Process and Chemical Engineering, and Theory.

This year's host location was German-Russian Institute of Advanced Technologies (GRIAT) located at one of the leading Russian universities the National Research Technical Tupolev University (KAI). GRIAT is a unique educational platform that unites German and Russian universities and companies, trains multilingual engineers with global engineering skills, encourages multinational research and development activities, and promotes cross-cultural understanding and friendship between Germany and Russia.

We thank all of you, the participants, for your involvement and cooperation in this conference.



Dr Andreas Hoeschen

German Academic
Exchange Service
Head of DAAD Office Moscow
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Professor Dr Albert Gilmutdinov
Rector of Kazan National Research
Technical University named
after A. N. Tupolev – KAI

DEAR COLLEAGUES AND PARTICIPANTS OF THIS THE CONFERENCE!

Kazan National Research Technical University named after A. N. Tupolev – KAI has the honor to host the 8th Russian-German Week of the Young Researcher.

The event is held on the basis of the German-Russian Institute of Advanced Technologies (GRIAT) which operates in a consortium with partner universities in Germany and with the organizational and financial support of the German Academic Exchange Service (DAAD).

Conferences of this format present us with this type of dialogue on science that enables us to build such type of a conversation about science that helps to form a steady interest in knowledge, increases the prestige of science, promotes innovation achievements, strengthens the links between science and education, science and business, and, most importantly, encourages involvement in research activities for talented youth.

I express my gratitude to our colleagues: they support active work on cooperation of the two countries. What are we doing here at the university? We are trying to jointly train a new generation of scientists in a climate of mutual support and respect. And such events, of course, are the key to establishing relations between people as well as joint work on projects.

The conference raises a wide range of issues of conservation and transformation of energy. These issues are acute for modern society. The conference presents reports on thermoelectric materials, carbon fuels and solar energy as well as a number of new technologies that scientists believe will help prevent energy shortages. Research organizations and higher education institutions of both countries will present funding programs and platforms for both Russian and German graduate students. The fundamental principle of the whole event is to promote cooperation as well as the creation and expansion of the Russian-German research community.

For the Republic of Tatarstan, where the leading industries are oil production and petrochemicals, the topic of this the conference is extremely specially relevant. Our country is rich in oil and gas, so Russia is therefore a little behind in the study of storage and processing of chemical energy. But it is obvious that renewable energy is the energy of future. It is obvious that renewable energy is the energy of the future. I really want this direction of research to be intensively developed in our university after this the conference.

I am sure that this event will give answers to all important questions.



DEAR ORGANIZERS, PARTICIPANTS AND GUESTS OF THE 8TH RUSSIAN-GERMAN WEEK OF THE YOUNG RESEARCHER,

It is a great honor for me to greet you here in Tatarstan, a place where significant all-Russian and international events were held several times, demonstrating industrial, scientific and educational capabilities of the Republic.

KAI is a university with a glorious history. It is known far beyond Tatarstan and Russia. Established in 2014, the German-Russian Institute of Advanced Technologies is actively developing the basis of the university. Being the largest educational project between Russia and Germany, GRIAT is an excellent example of successful interaction between Russian and German universities and companies.

The German-Russian Institute of Advanced Technologies has graduated more than 120 students. They are highly qualified specialists who received two diplomas; a Russian diploma of KNRTU-KAI and a German partner university diploma. They are employed at the leading enterprises of Tatarstan and continue their research in postgraduate studies. They are entrusted with the revival of the greatness of the engineering school. Moreover, the German-Russian Institute of Advanced

Technologies is a link with the industrial sector: there are three working Siemens AG laboratories as well as several engineering centers on the basis of the GRIAT. Regional and international forums aimed at popularizing engineering education are also being held there. Collaboration with the leading universities, development of joint research in the field of energy is one of the priority activities of the GRIAT and the industry of the Republic of Tatarstan.

I am absolutely confident that cooperation of the two countries will expand in the future, and this will be facilitated, among other things, by the Week of the Young Scientist. Within these few days, young scientists from Russia and Germany will discuss relevant issues of concern to the world community – preservation and transformation of chemical energy as well as technologies that will prevent energy shortages.

I encourage all participants to work fruitfully, to expand the scope of business contacts and to implement all the plans. I wish you success in all endeavors! I hope that Tatarstan and Kazan will become places where you will always be glad to return!



Rustam Minnikhanov
President
of the Republic of Tatarstan





Michael Dobis

Head of the Unit
of Science and Research,
German Embassy Moscow

DEAR PROFESSOR GILMUTDINOV, DEAR MR MÜLLER, DEAR MRS KOWOL-SANTEN, DEAR MR HOESCHEN, LADIES AND GENTLEMEN!

On behalf of the German Embassy in Moscow I am pleased to welcome you to the 8th German-Russian Week of the Young Researcher.

Since 2011, the Week of the Young Researcher has been bringing together academics from Germany and Russia to exchange ideas about challenges in various fields of science. It provides an opportunity to get to know new outstanding research results and approaches. It also allows the professional exchange between scientists – especially young researchers – from Germany and Russia. It is thus an inspiration for new connections and ties. The scientific cooperation between Germany and Russia is gaining dynamics and intensity.

This week has become possible due to the fruitful collaboration of very different partners. It is therefore one of the best examples for the variety of our bilateral cooperation in science and research:

- The German House of Science and Innovation in Moscow bundles the expertise of the numerous German scientific organizations and actively promotes new cooperation. It provides a platform for the cooperation between German and Russian institutions in science, research and innovation with a wide range of activities.
- The German Academic Exchange Service DAAD is the largest German organization supporting international academic co-operation and a very active partner and promotor of our bilateral relations.
- The German Research Foundation DFG awards the best researchers with funding and gives them the means and freedom necessary for successful research. One of its key objectives is the advancement of early career researchers. There-

fore this week would not be possible without the impact of DFG!

- The Kazan National Research Technical University (KNITU-KAI) is a founding partner of the German-Russian Institute of Advanced Technologies (GRIAT), also plays a vital and active role this week. The GRIAT is without any doubt one of the most visible and most successful cooperation projects in our science relations.
- Last but not least I would like to point out the support of the economic community. Siemens, a global powerhouse in the true sense of the word, has funded three laboratories at the KNITU-KAI, and it is hosting a special section „Science – Business – Innovation“.

With all this support and input, this week is an important contribution to our bilateral relations in science, research and innovation. It takes place in the run-up to a special event: The German-Russian year of Cooperation in Higher Education and Science 2018-2020. The aim of this thematic year under the patronage of the German and the Russian Foreign Ministers will be to further promote the various strands of our science relations and to promote and support the formation of new initiatives.

We want to intensify our collaboration in this area. Because science and research not only help us to overcome global challenges, they also promote exchange and dialogue across countries and cultures, as they rely on the universal language of knowledge gaining. On this note I wish you all an exciting week with many new encounters, stimulating conversations and new insights!

DEAR MS FAZLEEVA, DEAR RECTOR GILTMUDINOV, DEAR DR KOWOL-SANTEN, DEAR MR DOBIS, DEAR PARTICIPANTS OF THE "8TH GERMAN-RUSSIAN WEEK OF THE YOUNG RESEARCHER"

It gives me great pleasure to welcome you all to this year's "week" on behalf of the DAAD, the German Academic Exchange Service. First of all I would like to thank very warmly our host, the German-Russian-Institute of Advanced Technologies at the Kazan National Research Technical University. We highly appreciate your manifold contribution to this outstanding Russian-German science event, which already for the second time in its history takes place here at 'Tupolev'-University.

From the DAAD's perspective, this is very fitting, of course. Over the last two decades, Kazan National Research Technical University with its ever-growing commitment to internationalisation and to academic exchange with Germany has become an important partner for German universities in the Russian Federation. The DAAD has supported this mutually beneficial development right from the beginning through various scholarship programmes for students and researchers and project funding for university collaboration. Particularly, we are very happy to be able to run two collaborative scholarship programmes – named after "Nikolai Lobachevsky" and "Evgenij Savojiskij" – with the Republic of Tatarstan. These joint efforts helped lay the groundwork for the productive academic relationship we now see flourishing between German universities and their counterparts in Tatarstan in general and the Kazan National Research Technical University

in particular. In 2014 at the Kazan National Research Technical University, the "German-Russian Institute of Advanced Technologies" (GRIAT) was established based on a partnership agreement with Otto-Von-Guericke-University Magdeburg and Ilmenau University and supported by the DAAD. Subsequently the University of Kaiserslautern and the Technical University Braunschweig joined in and Siemens became an industry partner who contributed significantly to GRIAT's lab equipment. The expansion of the GRIAT-network is ongoing, its objectives are ambitious and it shows what can be achieved by sustained collaboration of a wide range of stakeholders from Germany and Russia. It sets a promising example not only for the international education of engineers but also for the German-Russian partnership in science and innovation.

Against this background GRIAT is simply an ideal host for this flagship event of the "German Centre for Research and Innovation" – the initiative of all Moscow based German Science organisations which promotes closer cooperation between Russian and German scientists and at the same time strives to facilitate a wider outreach of their joint endeavours. So, thank you very much again for your kind hospitality!

In order to attract scientists – regardless, if young or middle-aged – to an event outside their professional obligations, above all, the topic has to be cutting edge. I would like to thank the German



Christian Müller

Deputy Secretary General
of the German Academic
Exchange Service, Bonn



Research Foundation very much for having taken the lead in this regard. “Chemical energy storage and conversion” points to one of the major global challenges we are facing today. New ideas how to store energy much more efficiently and ensure its future supply are widely considered pivotal with a view to unprecedented and steady rising global energy demand. The linkage to addressing climate change is obvious and we all can easily agree that it requires global cooperation to find innovative solutions to such a global challenge. However, only the scientists themselves can deliver the crucial new knowledge. Therefore, scientists have to be able to share their expertise without stopping at borders. It lies at the heart of the DAAD’s mission to support this international circulation of ideas, which benefits us all.

The “German-Russian Week of the Young Researcher” brings together German and Russian scientists, senior researchers and those, who are just at the very start of their academic career. So, I am more than delighted that this year research-

ers from German universities, Helmholtz-Centres and Max-Planck-Institutes who are all highly distinguished experts in the topical field of our event have been willing to take the time to come to Kazan and to contribute to the event.

The “Week” aims to create a unique cross-border forum to disseminate and discuss advanced scientific approaches and fresh insights with a new thematic focus each year. In this respect, it is a one-off event. Nevertheless, it offers the opportunity for long-lasting inspiration and further academic engagement. As to that, I would also like to recommend visiting the Science Café on Wednesday where the “German Centre for Research and Innovations” and its organisations will provide information about support and funding for German-Russian science collaboration.

I thank everybody for participating, especially those of you who undertook a long journey – and I hope that all of you will enjoy and make the most of the event!

DEAR RECTOR GILMUTDINOV, DEAR MR DOBIS, DEAR MR MÜLLER, LADIES AND GENTLEMEN, DEAR PARTICIPANTS,

It is a great pleasure for us that you have accepted the invitation of the joint initiative of the German Academic Exchange Service (DAAD) and the Deutsche Forschungsgemeinschaft (DFG) under the auspices of the German Centre for Research and Innovation in Moscow. I am pleased to welcome you on behalf of the German Research Foundation to the “Eighth Week of the Young Researcher”!

“Week No 8” in this title implies that this conference stands in a line of tradition. In fact, this programme was inceptioned during the German-Russian Year of Science in 2011/2012, which led to an annual revival of a very old tradition in German-Russian cooperation. Namely, in the 1920s, the DFG’s predecessor organisation, together with the Soviet Academy of Sciences, organised joint science weeks. These bilateral research weeks, which were conducted in the natural sciences (1927), in history (1928), in engineering sciences (1929), and in medical sciences (1932) proved to be an outstanding cooperative instrument. In the spirit of those old days, the “German-Russian Week of the Young Researcher” also pays special attention to the next generation of researchers. We intend to provide early career researchers with a platform for exchange on research topics of global interest, with opportunities to network nationally and internationally, and – based on the interdisciplinary character of the event – with feedback and inspiration for their respective research questions from a wider scientific community.

Having focused on issues of energy, health, aerospace, history, mathematics, urban studies and biomedicine over the last years, this year’s topic encompasses various aspects of chemical energy storage and conversion including contributions from Materials Chemistry, Physical Chemistry, Process and Chemical Engineering, and Theory. Special attention is given to the challenges for improved materials and processes and their potential impact on existing and future applications and innovation.

Given the growing population and rising living standards, the world is faced with an increasing demand for energy. In fact, fossil fuels are not a sustainable resource and the natural reservoirs are limited. In all future scenarios, chemical energy storage and conversion plays a vital role to satisfy the increasing demand for energy. Innovative concepts offer opportunities for new processes without increasing harmful emissions of carbon dioxide (CO₂).

Chemical research is the key for a fundamental understanding of energy conversion and it opens the door to a broad range of future technologies. To name a couple of them: Sustainable solar energy technologies are the basis for harvesting energy from sunlight. Innovative fuel cells can efficiently convert fuels and exploit new energy sources. New and robust catalysts based on elements that are more abundant will pave way for more efficient processes. Thermoelectric materials, which generate electricity directly from heat, can also be used



Dr Johanna Kowol-Santen

Deputy Head of the Department
of Scientific Affairs
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Bonn

for energy conversion applications. Next-generation batteries with higher capacities and beyond lithium will flexibly store and transport energy, thus enabling higher degrees of mobility.

There is no doubt that this broad range of research questions is of high interest to many researchers worldwide. The DFG with its annual budget of more than 3 billion Euros, finances and supports a large number of very interesting and often interdisciplinary projects in this field of research at German universities and research institutes with funding instruments ranging from individual grants to coordinated long-term programmes such as Research Training Groups or Collaborative Research Centres.

To name just a few examples, we currently finance a project called “Fuels Produced regeneratively through Light-Driven Water Splitting – a DFG Priority Programme coordinated at the Technical University of Darmstadt and with projects spread all over Germany. Furthermore, we support a cluster of excellence on “Unifying Concepts in Catalysis” at the Technical University of Berlin jointly with the Fritz Haber Institute of the Max Planck Society and the Max Planck Institute of Colloids and Interfaces in Potsdam. Also, the DFG-funded Giessen based Research Training Group “Substitution of Material for Sustainable Energy Technologies” currently ventures to explore new materials based on abundant elements, a step necessary for technologies like high-efficiency photovoltaics, large-scale rechargeable batteries or intelligent glazing.

This list of examples is not complete without mentioning the Collaborative Research Centre “Heterogeneous Oxidation Catalysis in the Liquid Phase – Mechanisms and Materials in Thermal, Electro-, and Photocatalysis” led by Professor Dr. Malte Behrens at the University of Duisburg-Essen. These are, of course, only a few current examples, but they show that we, as a global society, have recognised the relevance of the topic and its knowledge-generating potential.

When it comes to German-Russian cooperation, chemistry profits tremendously from the annual bilateral DFG calls with the Russian Foundation

for Basic Research and the Russian Science Foundation. Those thematically open calls foster long-term cooperation in chemistry between Russian and German scientists. Russia is and stays one of the most important cooperation partners in chemistry, which is proven by the various published results from DFG-funded projects. We have been promoting German-Russian cooperation for many decades, since 2003 even with our own DFG-Office in Moscow. In the beginning of this century, around 2006, the DFG teamed up with the Russian Academy of Sciences to enhance delegations visits and joint chemistry conferences in order to foster the already existing academic ties in the field of chemistry research between our countries dating back even to the Soviet times. In 2007, renowned Russian chemists from Moscow, Yekaterinburg and Novosibirsk traveled to Bonn, Mainz, Munich and Berlin. In 2008, in return, a delegation of German chemists, among them several DFG review board members, visited Moscow and Yekaterinburg. This culminated in a German Russian Conference on “Nanomaterials in Chemistry” in Moscow in 2010 and a second conference at the Freie Universität Berlin on “Fundamentals and Applications of Nanoscience” embedded in the German Russian Year 2012.

Obviously, the intense scientific exchange between Russia and Germany is a long practiced reality, which can be retraced to the hour of birth of modern chemistry. This might be an inspiration and a reason enough for us all to actively participate in these upcoming days – a time that promises to be a week full of interesting presentations and discussions. I am convinced that we will be able to shape the future in science and in other areas of society, if we continuously bring young and senior scientists with international academic backgrounds together and provide a platform for an intense exchange of ideas.

I want to express my gratitude to the rector of the Kazan National Research Technical University named after A.N. Tupolev (KNRTU-KAI), Prof. Albert Kharisovich Gilmudinov. With the German-Russian Institute for Advanced Technologies (GRIAT) as our co-organizers, we can rely on professional partners when it comes to

fostering German-Russian scientific cooperation. Thank you very much for jointly organizing and supporting this project.

I am sure that our week of scientific exchange in this particular field of research perfectly adds value to the scientific community in Kazan as such, with Kazan being a scientific location known for its strong focus on chemistry. This encompasses various institutions all over Kazan such as the Alexander Butlerov Institute of Chemistry at the Kazan Federal University or the Arbuzov Institute of Organic and Physical Chemistry of the Kazan Scientific Centre of the Russian Academy of Sciences, but also a strong business sector in chemistry. The city is considered the birthplace of organic chemistry due to works by Aleksandr Butlerov, Vladimir Markovnikov, Aleksandr Arbuzov, as well as the birthplace of electron spin resonance discovered by Evgeny Zavoisky. And if you ever wondered about the etymology of the element ruthenium – it was discovered in 1844 by Karl Ernst Claus, a Baltic German chemist, who lived and worked as a professor in Kazan and named the element in honor of Russia.

Against this background, it seems like a perfect coincidence that the United Nations have proclaimed

the International Year of the Periodic Table of Chemical Elements in 2019 and thus honouring its 150 years of existence. It is rumoured that the Russian Dmitri Mendeleev and the German Lothar Meyer – who published his work on “Die Natur der chemischen Elemente als Funktion ihrer Atomgewichte” just one year after the publication of “The periodic law” (1869) by Mendeleev – both got the impetus for their subsequent independent research on the Periodic Table of Elements while jointly attending the first international congress on chemistry in Karlsruhe in 1860.

Finally, I would like to thank the German Embassy for continual support regarding this format. You have long recognised that these scientific meetings foster research cooperation and make a valuable contribution to developing trust and partnerships among the early career researchers and future generations of scientists from both our countries.

Having said this, I wish you and all of us a successful eighth German-Russian “Week of the Young Researcher”. In addition, be assured, in my function as Head of Chemistry and Engineering Sciences Division at the DFG, I am especially looking forward to new insights in our research field. So let’s enjoy the week!



PARTICIPANTS OF THE WEEK OF THE YOUNG RESEARCHER



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Controlling Activity and Selectivity for CO₂ Methanation on Highly Active Ru/TiO₂ Catalysts

Ali M. Abdel-Mageed, K. Wiese, Ashlee K. Hauble, R. Jürgen Behm
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The reduction of CO₂ to methane (CO₂ + 4 H₂ => CH₄ + 2H₂O) is a promising reaction for the decentralized storage and distribution of electric energy produced from renewable resources, known as the “power-to-gas” (P2G) concept.^{1,2} This way, H₂ produced from surplus electrical energy can be converted to CH₄, which can be easily stored and distributed using the standing natural gas grid.²

Oxide-supported Ru nanoparticles, in particular Ru/TiO₂, are among the most active catalytic systems for the methanation of carbon dioxide at moderate temperature range (190–300°C).³ A major setback for large scale applications is, however, the parallel consumption of H₂ via the undesired RWGS reaction (CO₂ + H₂ <=> CO + H₂O) which results in an undesired consumption of H₂ fuel.⁴

Recent studies in our group revealed that the specific surface area (SA) of TiO₂ strongly affects the metal-support interactions (MSI) in Ru/TiO₂ catalysts and thus their activity for CO₂ methanation and also the selectivity for the selective methanation of CO in CO/CO₂ mixtures.⁵ While Ru/TiO₂ catalysts with SA below 200 m²g⁻¹ are only active for methanation over a wide range of temperatures (190–350°C), Ru/TiO₂ with high surface area (>200 m²g⁻¹) start to catalyze the RWGS reaction already at about 230°C. In this case the RWGS becomes dominant at the higher temperatures and CO₂ methanation is simultaneously and completely suppressed.⁵

Here we report on a high-temperature modification of the catalyst support, which affects the performance of these catalysts. When operating the high SA catalyst at higher temperatures (≥350°C) and returning to lower temperature, this catalyst

was found to be active for the RWGS even under these conditions. On the other hand, the catalysts with SA <200 m²g⁻¹ become even more active for CO₂ methanation at 190°C after being operated at higher temperatures. These observations point to irreversible structural and possibly electronic changes of the Ru/TiO₂ catalysts, which strongly affect their catalytic performance. This hypothesis will be discussed based on kinetic and in situ infrared measurements, in combination with detailed catalyst characterization by a variety of different techniques before and after reaction at different temperatures.

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Solar Chimney with Heat-Accumulating Layer

Objectives. Natural ventilation systems are the oldest «green» technology, which can provide the required parameters of indoor microclimate without using electricity. To intensify the air exchange, it is possible to use thermal inducement of air. Systems with radiation heating of ventilation ducts (solar chimneys) are the most prevalent nowadays. The first solar chimney was developed by NK Bansal [1]. Later, more complex systems were developed by T Tongbai [3], OK Ahmed and AS Hussein [2]. The article offers improved design of the exhaust ventilation duct with heat-accumulating layer. The possibility of thermal energy accumulating is based on physical (melting and crystallization) and chemical (adsorption) processes with the release and absorption of heat. The heat-accumulating layer is a container filled with phase change material (PCM) – technical grade paraffin wax. The melting point of this material can vary in a wide range from -9 to 100 °C. PCM possess high latent heat, they are chemically inert and have unlimited lifetime.

Methods. To determine the desired melting point of PCM, mathematical modeling of internal natural convection was carried out using the CFD software, based on the finite volume method with unstructured mesh.

Results. The article presents selection method of phase change materials for solar chimneys.

Conclusion. The application of heat-accumulating layer in systems with radiation heating of ventilation ducts can ensure stable air exchange during the day, including in the evening hours.

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Influence of Temperature and Electrolyte Concentration on the OER Catalytic Activity of NiFe LDH

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Water splitting electrocatalysis research conducted in the last years focuses mainly on the development of highly active electrocatalysts for both anodic and cathodic reactions. Oxygen evolution reaction (OER) is considered the limiting part, high overpotential being required to evolve oxygen. NiFe LDH is known to be the most active non-noble metal based OER electrocatalyst in alkaline environment.[1] Beside being active, the stability of the catalyst is also crucial for development of alkaline water electrolysis.[2] Alkaline electrolyzers use high concentrated alkaline solution ($\sim 30\%$ wt.) and operate at higher temperatures (~ 80 °C) under high current densities (~ 500 mA cm^{-2}). At higher current density, due to the high mechanical stress induced by bubble

formation, the stable immobilization of the catalyst on the electrode becomes very important. Recently we introduced polybenzoxazine as carbon precursor for stable immobilization of powder catalysts on the electrode surface.[3] Longterm experiments performed at 200 mA cm^{-2} in 5 M KOH at 60 °C show that NiFe LDH transforms in 100 h into a mixture of NiO and Fe_2NiO_4 . [4] These transformations were not reported previously, suggesting that the environmental conditions used for the catalyst evaluation impact its structure and thus its electrocatalytic performance.

In the present work, we investigated the chemical stability of NiFe LDH in KOH solutions having different concentrations and under higher temperatures. The chemical transformations evaluated us-



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ing techniques like X-Ray diffraction (XRD), Fourier transformed infrared spectroscopy (FT-IR), Raman spectroscopy and Transmission electron microscopy, as well as their influence on the electrochemical OER activity will be presented.

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Professor Evgeny Antipov

is a graduate of the Lomonosov Moscow State University (1981). He obtained a PhD and Doctor of Sciences degrees in 1986 and 1997, respectively. Since 1981 he has been working at the same University, beginning as a scientific researcher and later working as a full professor and the head of the electrochemistry department. Professor Antipov's research interests are mainly focused on design, synthesis, crystal structure and characterization of advanced inorganic materials for energy application: superconductors, electrode materials for batteries, fuel cells and etc. He has received several awards for the scientific achievements. Professor Antipov authored 370 publications. He has a h-index of 36 (Scopus) and over all citations over 6000. Evgeny Antipov is an elected Corresponding member of the Russian Academy of Sciences and as a member of the Academia Europaea.

Alkali and Transition Metal Fluoride-phosphates as Perspective Cathode Materials for Metal-Ion Batteries

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The ever-growing demand for portable energy in various fields puts forward new challenges to rechargeable battery technologies in improving specific energy and power, life and safety. The battery performance is critically governed by the properties of the cathode material. Fluoride-phosphates of transition metals with A_xMPO_4F ($A = Li, Na, K; M = V, Fe, Co$) formula take several advantages over existing oxide cathode materials: a substantial increase in operating voltages and much faster kinetics.

A distinctive structural feature of these materials is the presence of dangling oxygen atoms (bonded to P and alkaline cations, but not included into the octahedral coordination of transition metals). These oxygen atoms can determine the mechanism of the structure transformation during charging and even trigger the undesirable cation intermixing. Different activities of the alkali positions surrounded by a distinct number of the dangling oxygen atom can explain the striking difference between desodiation mechanisms in Na-ion and Li-ion cells of a layered Na_2FePO_4F cathode

material. Its counterpart, Li_2FePO_4F , was found to undergo a severe cation intermixing during charging to compensate a strong underbonding of the dangling oxygen atoms upon removal of the Li^+ cations from their coordination sphere.

We designed and prepared a new vanadium-based $AVPO_4F$ ($A = Li, K$) cathode material adopting a KTP-type framework with excellent rate capability. The material showed remarkable capacity retention in Li-ion cells at 40°C maintaining more than 75% of the initial specific capacity. It can also reversibly incorporate Na^+ and K^+ ions unveiling rapid kinetics and preserving the host structure. The alkali ion diffusion coefficients measured using the PITT technique were the lowest for Li^+ ($10^{-12} - 10^{-14} \text{ cm}^2/\text{s}$) and highest for K^+ ($10^{-11} - 10^{-12} \text{ cm}^2/\text{s}$) making $AVPO_4F$ a promising candidate for metal-ion batteries.

Our current activities on transition metal fluoride-phosphate based cathode materials for metal-ion batteries will be reported with a particular focus on the interrelation between crystal structure peculiarities and electrochemical properties.

Au/ZnO Catalysts for Methanol Synthesis in Chemical Energy Storage Concepts

Methanol synthesis from CO_2 and H_2 generated from renewable energies via the reaction $\text{CO}_2 + 3\text{H}_2 \rightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}$ (1) is an attractive option for storing excess electric energy, e.g., from wind power and photovoltaics, and at the same time reduce CO_2 emissions. To avoid long distance transport of excess electric energy it would be desirable to operate these processes locally, in a decentralized concept. This results in two problems compared to the large-scale production of methanol from syngas: First, for small-scale operation the reactor design and process conditions should be as simple as possible. Second, the process should be able to tolerate very dynamic process conditions, which are dictated by the fluctuating nature of renewable energy sources. Both of these conditions preclude a simple downscaling of current industrial processes and catalyst concepts.

We have recently demonstrated that oxide-supported Au catalysts, specifically Au/ZnO catalysts, are promising candidates for the selective MeOH formation from CO_2 and H_2 [1,2,3]. Under moderate reaction conditions at pressures of 5–50 bar and reaction temperatures of 220–240°C, the catalytic performance of Au/ZnO catalysts in the CO_2 hydrogenation to MeOH surpasses that of commercial Cu catalysts. This includes both a higher activity for MeOH formation and a significantly higher selectivity for this process as compared to the competing reverse water-gas-shift reaction to CO and H_2O .

So far, however, there is little information on the functioning of these catalysts on a molecular scale, which is crucial for the further optimization of the catalysts and reaction conditions to realize the above concepts. This is the topic of the present talk, where I will present results of recent studies combining kinetic and in situ / operando spectroscopy measurements, performed at pressures between ~1 mbar and 50 bar, where the latter corresponds to technical conditions [4]. Insights from these combined measurements will be discussed.

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Jürgen Behm

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R. Jürgen Behm studied chemistry at the Ludwig-Maximilians-Universität in Munich and received his PhD in Surface Science in the group of Prof. G. Ertl. After post-doctoral research in the IBM Research Laboratory in San José / USA, he focused on the new topic scanning tunnelling microscopy. This was also the basis for his habilitation in Physical Chemistry at the LMU in Munich. After working as a group leader at the Fritz-Haber-Institute of the Max-Planck-Gesellschaft and as Associate Professor at the LMU Munich, he became Full Professor and Director of the Institute of Surface Chemistry and Catalysis at Ulm University in 1992. His research (>620 publications, H: 88) focuses on the microscopic understanding of surface processes in heterogeneous catalysis and electrochemistry/-catalysis.





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Malte Behrens is a Professor of Inorganic Chemistry at the University Duisburg Essen, and Vice-Dean at the Faculty of Chemistry at UDE Germany. He studied Chemistry and received a Diploma at the Christian Albrechts University of Kiel (CAU). In 2002, he wrote his PhD thesis there. Between 2008 and 2014, Malte Behrens was the leader of the Nanostructure-Group at the Fritz-Haber-Institute of Max Planck Society, Department of Inorganic Chemistry. In 2013, he habilitated at the Technical University Berlin on "Materials Chemistry of Cu/ZnO-based Catalysts for Methanol Synthesis and Steam Reforming". Since 2018, Professor Behrens has been the spokesman of Collaborative Research Centre (CRC Transregio247) "Heterogeneous Oxidation Catalysis in the liquid phase" funded by the DFG.

Inorganic Materials for the Catalytic Generation and Chemical Storage of Hydrogen

Heterogeneous Catalysis is a key science for efficient chemical energy storage. In the so-called power-to-liquid approach, renewable electric energy can be converted into chemical energy by water electrolysis producing hydrogen. Hydrogen can be further processed and transformed into more feasible synthetic fuels like methanol in a subsequent downstream step. The efficiency of both steps is greatly determined by the nature of the (electro-)catalysts applied.

In the case of water electrolysis, the anodic half-reaction, the oxygen evolution reaction (OER), is the kinetic bottleneck. In alkaline electrolyzers, 3d transition metal oxides of the groups 7–10 (Mn to Ni) are attractive, because of their high activity and low costs. The potential of pure Manganese oxides seems limited by low stability and low electric conductivity, while mixed oxides of Co, Fe and Ni show interesting variation of the OER overpotential with composition x in $\text{Co}_{1-x}\text{Ni}_x\text{Fe}_2\text{O}_4$. [1] A similar behavior was observed for nanoparticles of $\text{CoFe}_{2-x}\text{V}_x\text{O}_4$. [2]

For utilization of hydrogen and CO_2 in methanol synthesis, ZnO_x -promoted Cu metal catalysts are among the most attractive catalyst materials. The

promoting effect can be understood based on the beneficial role of (partially) reduced ZnO_x for the activation of the formate intermediate. [3] For both reactions, potential avenues for catalyst optimization will be presented and discussed.

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Anode Materials for Sodium Ion Batteries

Wolfgang Bensch and Markus Krengel

For large scale energy storage devices, sodium ion batteries (SIBs) are an attractive alternative to lithium ion based batteries (LIBs). The main problem of SIBs is the lack of a suitable anode material. We identified the thiospinel CuV_2S_4 [1] and quasi-layered CuCrS_2 [2] as promising anode materials in SIBs exhibiting large specific capacities and an excellent cycling stability. For CuV_2S_4 , a revers-

ible specific capacity of 580 mAh/g was obtained in the 300th cycle. A Coulombic efficiency of 99% is achieved after the 3rd cycle. During Na uptake (discharge) first Cu^+ ions are reduced and expelled from the electrode as nanocrystalline elemental Cu which was evidenced by X-ray powder diffraction (XRPD). Increasing the Na content per formula unit leads to a full conversion of CuV_2S_4 with Cu

and V nanoparticles being embedded in a Na_2S matrix. The presence of Na_2S was evidenced by ^{23}Na magic angle spinning NMR experiments. At later stages of cycling elemental Cu partially reacts to form Cu_2S . The good electrical conductivity of $\text{Cu}/\text{Cu}_2\text{S}$ seems to be beneficial for superior cycling and rate capability. For CuCrS_2 a reversible specific capacity of 424 mAh/g is obtained in the 200th cycle. First Cu^+ is reduced to metallic nanoparticles and Na^+ is inserted in the host materials to form $\text{Na}_{0.7}\text{Cu}_{0.15}\text{CrS}_2$ as intermediate phase according to XRPD investigations. In the XRPD pattern of the fully converted material reflections of elemental Cu and Na_2S are observed, but no hints are found for the presence of elemental Cr. Synchrotron radiation based pair distribution function (PDF) anal-

ysis evidences the presence of nanoscopic chromium particles in the material.

The results of the investigation of the two materials are presented in the speech.

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Wolfgang Bensch studied Chemistry from 1973 to 1978 at the Ludwig Maximilian University of Munich. In 1983 he obtained his PhD at the LMU. Between 1984 and 1986, he was a research fellow at the University of Zurich, Institute for Inorganic Chemistry, and joined Siemens Company, Munich, in 1986. In 1993 he habilitated at the University of Frankfurt and stayed there till 1996 as a research fellow. In 1997 he obtained the professorship in Inorganic Solid State Chemistry at the University of Kiel. Professor Bensch is a member of the DFG review board 302 "Chemical Solid State and Surface Research" since 2012 and Spokesperson of this review board since 2016. He is also a member of the Cluster of Excellence "The Future Ocean" at the University of Kiel.

Electrochemical Noises of Pem Fuel Cells and Their Diagnostic Properties

Electrochemical noise diagnostic is used for studying corrosion processes in metal films, quality of passivation coatings and charging/discharging processes in electrochemical batteries. The main advantage of this method is the absence of any operation mode perturbation. In frame of the present work we apply the electrochemical noise diagnostics to one of the most perspective power source Proton Exchange Membrane Fuel Cell (PEMFC). The fluctuation-noise model taking into account features of charge transfer processes as well as fluctuation phenomena within PEMFC has been developed. Simulation result is in good agreement with the experimental results and small differences could be explained by the influence of the measurement equipment internal noises. The high volume of experimental data is accumulated for fluctuations of PEMFC cells and their stacks in different operation modes. It is established that fluctuation phenomena provide information about technical state of PEMFC and detect dry-

ing and flooding processes, non-uniform current distribution, etc. Long term tests for PEMFC stack was carried out within 1000 hour. It has been proved that the fluctuation parameters are stable and repeatable. The analysis shows that the spectrum of PEMFC stack fluctuation coincides in general with one of single cell and could be used to study physical and chemical processes therein. The obtained result allows to consider the electrical noises and fluctuation as perspective diagnostic tool for PEMFC.

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Novel Fluoride-Phosphate Based High-Energy Cathode Materials for the Next Generation of Rechargeable Batteries

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Performance of various battery-driven devices requires constant enhancement to meet the ever-growing demand and expectations and thus stimulating the development of next generations of batteries. A crucial element of the rechargeable battery is a positive electrode (cathode), which primarily defines the most of its functional and electrochemical properties and cost.

by ex-situ electron tomography. It follows a sequence of phase transformations characterized by small volume variation, though preserving the parent structure.

The materials support reversible de/insertion of Na⁺, K⁺ [2] and even Rb⁺ [3] ions. The full de/insertion of K⁺ in KVPO₄F occurs at the highest potentials comparing to Li⁺, Na⁺ and Rb⁺ exceeding 4.6 V vs K/K⁺, which considers KVPO₄F as the most high-voltage cathode material for K-ion batteries investigated so far.

The KTP-type “VPO₄F” framework showing reversible de/intercalation of four types of alkali ions opens up new prospects in designing polyanion-based cathodes for metal-ion batteries. The presentation will be focused on our recent results on KTP-type fluoride-phosphates considered as promising cathode materials for metal-ion rechargeable batteries.



In our group we recently perfected a novel series of AVPO₄F (A = Li, Na, K, Rb) cathode materials, adopting a unique KTiOPO₄ (KTP)-type structure, which enables excellent rate capabilities particularly demonstrated in Li cells [1]. A remarkable capacity retention of more than 75% of the initial specific capacity is maintained in Li-ion cells at 40C and an average potential of 4.0 V vs Li/Li⁺.

The material undergoes an interesting structural evolution upon cycling in Li-cell, examined

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Ionothermal Carbons for Energy-Related Applications

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Polymer electrolyte membrane fuel cells (PEMFC) are amongst the most promising energy conversion technologies today. Herein non-precious metal based catalysts such as Fe-coordinated nitrogen doped carbons (FeNCs) are very promising alternatives for Pt-based cathode catalysts.[1-3] The early reports on the application of such materials date back to the 1960's when Jasinski demonstrated that N-coordinated transition metals can be active sites for the ORR.[4]

The preparation of these catalysts was strongly optimized over the years; still they remain with harsh reaction conditions that complicate the selective formation of active FeN₄ sites. The employment of pyrolytic temperatures has been a dogma for the synthesis of FeN₄ sites, however coming with unfavorable side reactions.

We recently introduced a mild procedure, which is conservative toward the carbon support and leads to an active-site formation at low temperatures in a wet-chemical coordination step, essentially decoupling the preparation of NCs from the preparation of the active sites.

The key concept for the success is the so-called active-site imprinting into the NC before the involvement of iron. Active-site-imprinted NCs were synthesized employing Lewis-acidic Mg²⁺ salt in the carbonization. The obtained carbons with large tubular porosity and imprinted N₄ sites lead to catalysts with a half-wave potential ($E_{1/2}$) of up to 0.76 V vs. RHE (in halfcell tests) in acidic electrolyte after coordination with iron. The catalyst shows 4e⁻ selectivity and exceptional stability with a half-wave potential shift of only 5 mV after

1000 cycles between 0.3 and 1.0 V in O₂-saturated electrolyte. The X-ray absorption fine structure as well as the X-ray absorption near edge structure profiles of the most active catalyst closely match that of Fe(II)phthalocyanine, proving the formation of active and stable FeN₄ sites at 80 °C. Perspectively, the decoupling of carbonization and active site formation allows for transfer of nanochemically designed carbons, so far mostly employed for alkaline conditions, to the more relevant acidic conditions.[5]

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Sustainable Hydrogen Production via Ammonia Decomposition over Bi-metallic Iron Catalysts: Promotional Effect of Gallium and Cobalt

Bi-metallic surfaces have the potential to dramatically enhance the efficiency of catalytic processes that is often associated with their unique electronic and geometric properties.[1] This promoting effect is determined by the interaction of the involved metal species, which can be influenced by the synthesis recipe of a specific catalyst. In this context, one promising approach for synthesizing Fe-based bi-metallic compounds is the use of layered double hydroxides (LDHs) as single source precursor materials. A great advantage of these hydrotalcite-like compounds lies in their high flexibility in terms of chemical composition, which can be tuned by isomorphous cation substitution. This strategy allows the incorporation of a second metal like Ga or Co into the precursor with a high degree of homogeneity. Since iron has two accessible oxidation states in aqueous solution, it is furthermore possible to obtain nanostructured spinels by calcination of co-precipitated LDHs by adjusting the $\text{Fe}^{2+}:\text{Fe}^{3+}$ ratio. Substitution of Fe^{3+} with Ga^{3+} species was found to be highly beneficial for the ammonia decomposition activity of the resulting Fe/MgO-based catalysts.[2] An even greater promoting effect was

observed upon replacement of Fe^{2+} with Co^{2+} cations. Both the physicochemical and the catalytic properties of these new materials were systematically investigated to gain a deeper understanding of the key factors that affect the promoting effects.

Mesoporous Fe-Mg-Ga and Fe-Mg-Co based LDH precursors were successfully synthesized by co-precipitation using an automated synthesis workstation. This allows an accurate setting and monitoring of crucial parameters, including pH and temperature. Consequently, a controlled variation of the pH in small steps from 8.5 to 10.5 at a given composition and changes in chemical composition at the precursor stage clearly showed the high sensitivity of the resulting catalysts to the synthesis conditions.

In situ XRD investigations[3] in combination with TPR analysis indicated the formation of an intermetallic Fe_3Ga phase after reduction at high temperatures. Interestingly, a highly active $(\text{Fe-Ga})\text{Fe}_3\text{N}$ nitride phase is formed under working conditions. In apparent conflict with the principle of microscopic reversibility, the Fe-Ga bi-metallic catalysts were almost inactive in ammonia synthesis.[2] The incorporation of Co enhances the ammonia decomposition activity up to six times at 500 °C in comparison with mono-metallic Fe supported on MgO.

Properties of iron catalysts in the catalytic ammonia decomposition are strongly influenced by the composition, but also by the synthesis route and the exact setting of the synthesis parameters. By using LDH precursors, iron particles can be modified with Ga and Co, resulting in bi-metallic catalysts that are highly efficient in the sustainable generation of hydrogen via the ammonia decomposition reaction.



Cell Design Aspects in Lab Scale Electrocatalytic CO₂ Reduction Experiments

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Electrocatalytic CO₂ reduction could lead to a simple one-step process which is able to directly transform electrical energy from renewable sources to green carbon-based energy carriers and base chemicals from CO₂ and water. For this reason, electrocatalytic CO₂ reduction recently became a very active research field with currently several hundred publications a year.[1] As promising this technology is, electrocatalytic CO₂ reduction is still facing many challenges. For example, further improvement is needed with respect to increasing current density, catalyst stability and product selectivity.[2] While most of the research address the synthesis and testing of new heterogeneous catalysts, only little attention is paid to the design of cells and pitfalls related to determining correct

values for the electrode potential or other analytical parameters.[3] This presentation therefore will focus on issues related to the cell design for CO₂ reduction as well as the choice of materials/electrolytes.[4] Mitigation strategies for better experimental results will be discussed.

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Sunlight Driven CO₂ Valorization via Photocatalysis and Heterogeneously Catalyzed Glycolic Acid Upgrading

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The synthesis of value added products from CO₂ is attractive for two reasons. First, CO₂ as a greenhouse gas is converted and second, if sunlight is used as energy input for the conversion, the CO₂ emissions normally occurring during the production are omitted or greatly reduced. Two different projects are presented to achieve this goal.

In a first approach, CO₂ will be directly converted to value added products such as CH₄, CH₃OH or products containing more than one carbon atom via photocatalysis in aqueous CO₂-saturated solutions. To enable conversion with sunlight, a band gap engineering of the photocatalyst is often necessary (e.g. via composite materials or metal doping [1]). These bandgaps are then routinely characterized via UV-Vis spectroscopy using different mathematical and graphical methods for the evaluation [2]. It was found that the evaluation method used has a strong influence on the band gap determined and that careful choice of the method is necessary as the observed trend in band gap alteration can be dependent on the method applied (Fig. 1).

A second approach deals with the aqueous phase reduction of glycolic acid (GA), obtained as metabolic product of sunlight irradiated algae (*Chlamydomonas reinhardtii*), to ethylene glycol (EG). Here, different supported metal catalysts were investigated, indicating that Ru-based catalysts are most suitable under the reaction conditions investigated. Using a commercial Ru/C catalyst at 120 °C and 80 bar H₂-pressure 58% yield to ethylene glycol could be achieved in 55 hrs of reaction time (Fig. 2).

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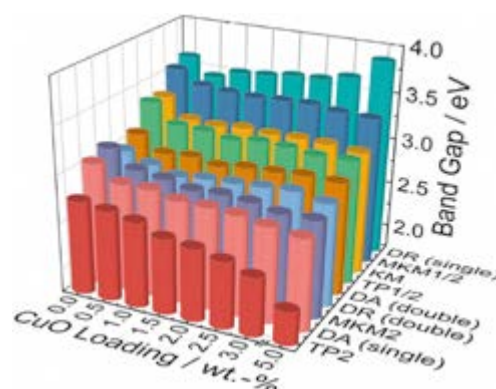


Fig. 1: Method and loading dependent band gap of CuO doped TiO₂ determined via UV-vis spectroscopy

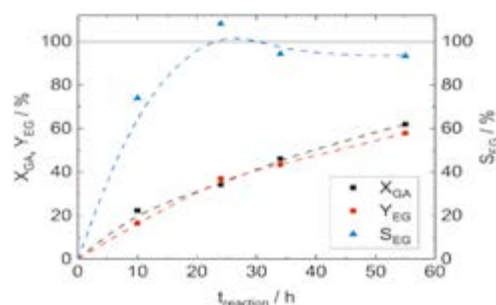


Fig. 2: GA conversion (X_{GA}), EG selectivity (S_{EG}) and yield (Y_{EG}) for the hydrogenation of GA at 120 °C and 80 bar H₂-Pressure

Carbon-Based Electrodes – a Black Prospect for a Bright Future

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Electrocatalysts for oxygen evolution and reduction reactions (OER and ORR) are key functional components for chemical energy conversion and storage devices respectively. To make this technology economically competitive, widely available and environmentally friendly, it is important to find alternatives to current electrode materials, which are based on scarce noble metals, typically based on platinum or iridium oxides.

Carbon based electrode materials are very promising candidates. Challenges are to increase the activity while maintaining their stability by preventing dissolution or corrosion.[1] Synthesis can be fulfilled within in an autoclave process to obtain conductive hydrothermal carbon (HTC). Variations of the synthesis conditions or the usage of nitrogen containing additives like urotropine influence the material properties and their performance as electrocatalysts which were systematically investigated.[2] Furthermore, the modification of HTC or conventional carbon materials like carbon nanotubes (CNTs) with transition metal oxides can enhance their activity tremendously. Different deposition and binding approaches were successfully developed to prevent leaching of the metal species to maintain their excellent electrocatalytic performance.[3,4]

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Multi-Electron Redox Electrode Materials for Li- and Na-Ion Batteries

The use of multi-electron redox materials is the most effective way to build new battery systems with higher energy densities, which are determined by both specific capacity and working potential. However, for a majority of known systems, their redox reactions take place through a single electron process, while true multi-electron reaction involves at least one atom per formula unit as a redox center, which undergoes valence changes by more than one electron.

Many families of transition metal oxides as well as transition metal polyanionic frameworks have been proposed as cathode materials for lithium-ion batteries during the past twenty years. Among them, manganese, nickel, vanadium-based materials can operate with multi-electron cationic redox reactions due to the presence of several stable oxidation states, thus leading to higher capacity. In the past years great hopes have been placed on the emergence of anionic redox for designing positive electrodes with a near-doubling of capacity. Recently, a new electrochemically active rock-salt-type nanostructured compound $\text{Li}_4\text{Mn}_2\text{O}_5$ has been prepared by

direct mechanochemical synthesis at room temperature with a discharge capacity of 355 mAh/g, which is the highest among the known lithium manganese oxide electrode materials ever reported [1]. Its exceptional activity arises from the participation of the $\text{Mn}^{3+}/\text{Mn}^{4+}$, $\text{Mn}^{4+}/\text{Mn}^{5+}$ and $\text{O}^{2-}/\text{O}^\cdot$ redox couples.

Many electroactive materials used in sodium-ion batteries have the capability to undergo multi-electron processes. Among them is $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}_3$, which can operate using $\text{V}^{3+}/\text{V}^{4+}$, $\text{V}^{4+}/\text{V}^{5+}$ and $\text{V}^{3+}/\text{V}^{2+}$ couples [2]. When cycled within the 1.0–4.5 V, its theoretical specific energy increases up to 600 Wh/kg, rivaling that of several lithium-ion battery cathodes [3]. The search for reversible and stable anionic redox activity in Na-ion batteries is in progress.

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Organometallic Electrode Materials for New Generation of Batteries

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At present, several conceptions of electrochemical energy storage devices are known. Most of them are based on inorganic active materials restricted by limited mineral resources, waste treatment processes, as well as large energy consumption in their synthesis. A possible next step in power sources development might be the creation of novel organic and metalorganic “soft” materials with designed functionality.

Among the advantages of organic compounds, one can mention the relatively low impact on the environment and wide scope of possible modulations of electrochemical properties by structural manipulations [1]. In particular, various functional polymers, such as conducting polymers with extended π -systems [2], and nitroxide radical tetramethylpiperidine-N-oxyl (TEMPO)-based polymers [3] are explored as potential cathode materials.

In this report, we discuss organic cathode materials based on π -conjugated polymer complexes of transition metals modified by TEMPO-type functional groups with potentially high capaci-

tance. We have tested two approaches, leading to the increase of electron and ion conductivity of organic materials. The first approach represents mechanical mixture of conductive polymers with redox-active polymers. The second approach implies chemical linkage of the redox-active centers to the polymer chain. As a result, we have demonstrated the possibility of create electrode materials with overall capacitance more than 80 mAh/g, capable to fast charge/discharge at currents more than 5 C, even at temperatures below -30°C .

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Micro-Macro-Porous Composite Materials for Sorptive Heat Storage and Cooling

Saving energy is an important aim of scientific effort in the last decade, observing a growing world population and a decline of fossil primary energy carriers. A remarkable part of energy is used for heating and cooling purposes. Savings can be realised in this field by the technology of sorptive heat storage and sorptive cooling, where the involved energetic contributions of water ad- and desorption processes are used.

Zeolites and MOFs (metal organic frameworks) are promising candidates for implementation in sorptive heat storage and sorptive cooling applications due to their high adsorption enthalpy and/or water uptake capacity.[1,2] For taking advantage of zeolites and MOFs in the mentioned applications, it is essential to maintain a sufficient transportation of mass as well as heat into/out of the active material, which cannot be provided in a packed bed of small crystals. Therefore we favour the manufacturing of layers

of zeolites/MOFs on cellular materials (such as ceramic or metal foams), which offer high specific surfaces for layer formation and allow heat transport via the foam struts. This also fosters to avoid thermal hindrance of further adsorption and termination of the process.

For heat storage purposes we optimize the performance of zeolite materials, especially zeolite 13X, Y and chabazite by ion exchange in order to exploit the contribution of hydration enthalpy of the implemented cations. The modified zeolites are coated on optimized (porosity, heat conductivity) cellular alumina foams or on metallic cellular structures by a binder based route. In addition, composites are made by direct crystallisation and post-synthetic modification.

MOF materials show excellent water adsorption characteristics for sorptive cooling purposes. Here MOF materials like MIL-100(Fe), Al-Fumarate, CAU-10 or HKUST-1 are processed using a binder based coating route for cellular ceramic or metal foams. Also direct crystallisation comes into use on specially pre-treated cellular ceramics using static solvothermal synthesis conditions[3,4] or performing a novel dynamic synthesis approach. We discuss the manufacturing of selected micro-macroporous composite materials and their characteristics in the focus of the above mentioned applications.

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Design of Catalysts for Carbon Dioxide Valorization under Mild Conditions

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Increase in the level of carbon dioxide emissions leads to climate change. But at the same time, CO₂ is found to be a useful C1 building block for synthesis if in small molecules, such as: CH₄, CO, HCOOH, CH₂O, CH₃OH [1]. These molecules are desirable for energy storage (methane, methanol), synthesis of monomers and CO is widely used for Fischer–Tropsch process. However, direct chemical and electrochemical reduction of carbon dioxide still has low selectivity and efficiency [2]. In this work, the dependence on CO₂ electroreduction efficiency from structure of active sides in case of nitrogen-doped carbon nanotubes was studied. It is shown that increasing of electron density on pyridine-type nitrogen atoms increases yield of highly reduced methane and methanol. Also, the presence of hydrogen donor groups reduces over-potential up to 500 mV which is explained by the formation of adsorbed intermediates, stabilized by hydrogen bonds and containing more activated carbon atom. The study of mechanisms was performed using DFT method with B3LYP hybrid functional. The mechanism of electrochemical reduction, explaining catalytic effect of side groups was presented. As a model catalyst, N-aryl-hetero-

cycle grafted carbon nanotubes were used, their possibility to reduce carbon dioxide was shown using CV and GC.

Also, possibilities of development of novel non-precious metal complexes based catalyst were studied using mechanistical analysis. It was shown, that the most efficient processes in mild conditions can be achieved using pincer-ligand chelated cobalt and nickel complexes. Dependence of Ea of one-step CO₂ molecule activation process of molecular descriptors were studied. Increasing cone angle of ligands with metal-to-ligands bond strength decreases overpotential and increases faradaic yield. Obtained results can be used for further development of heterogeneous and homogeneous catalyst for CO₂ valorization.

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A Local View on Cu/ZnO/Al₂O₃ Catalysts for Methanol Synthesis

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Methanol is considered a prospective key compound for chemical energy storage. This molecule can be produced over Cu/ZnO/Al₂O₃ catalysts via the hydrogenation of CO₂. The origin of the activity relies on the synergism between Cu and ZnO, but details on their active phases are still debated. [1-3] The performance of these complex catalysts is influenced by local alterations on the nanoscale, which are often overlooked by integral and sample averaging techniques. Insights into the local structure of materials can be obtained by transmission electron microscopy (TEM).

This contribution focuses on TEM descriptions of the nano- and mesoscale of a copper based catalyst for methanol synthesis under static vacuum and dynamic feed conditions. In depth TEM investigation revealed a ZnO overlayer on top of the Cu nanoparticles after reductive activation.[4] The formation of this overlayer is based on the occurrence of strong-metal support interaction (SMSI) between Cu and ZnO. It further seems to be of paramount importance in the catalytic process and may tune the nature of the active phase. Details on the evolution of this ZnO overlayer during reductive activation and methanol synthesis helps to improve the level of understanding. As we will show the formation of the ZnO overlayer depends on the composition and activation temperature. This overlayer is prone to thermodynamic ageing during methanol synthesis, which can be correlated to the deactivation of this catalyst.[5] In addition, in situ TEM images can support the picture of a dynamic catalytic system.

In conclusion, the results demonstrate how local views into heterogeneous catalysts can enhance the information depths and understanding.

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Production and Use of Biogas as an Alternative Source of Energy

A variety of renewable resources of energy (sun, wind, water etc.) can hardly surprise anyone nowadays. However, some of such resources are not very well investigated and thus may have a significant potential for future. Moreover, we all have a special relation towards one of energy resource, which flows under our feet and is called wastewater. [1-3] There are three ways known to obtain energy out of waste water – anaerobic fermentation, heat pumps and reverse electrodialysis. Waste water of biological and chemical factories has a high concentration of organic compounds. A traditional system of biological treatment requires significant costs and energy consumption. Water consumption in cubic meters per one ton of production is reducing that result in growth of pollutants concentration in waste water. Only a combination of anaerobic and physical and chemical methods of treatment provides proper treatment quality for waste water with irregular and high concentrations of COD and fat (which can be hardly removed by means of aerobic treatment). [1,2]

The process of treatment is performed by means of methanogenic bacteria that are presented in anaerobic reactors. This method proved to be re-

sistant to both to sharp rise or fall of COD concentrations in waste water due, causing no biomass destruction. The technology was implemented in 7 factories. The biogas to be produced has only slight differences from natural gas in percentage ratio of methane and carbon dioxide. That is why it can be used for the same purposes. Heat productivity of biogas depends on methane concentration and values at 5000–6000 kcal per cubic meter (25–28 MJ per cubic meter). The most efficient solution is to use biogas for combined production of electric and heat energy. [3]

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Development of New Proton Conductive Membranes for Pem Fuel Cells

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The fuel cell represents a promising way of generating electrical power from a variety of fuels, which converts the chemical energy of a fuel and oxidant directly into electrical power. Polymer electrolyte membrane fuel cells (PEMFC) are an environmental-friendly and high efficient alternative of conventional energy sources [1-2].

A key component of PEMFC is a proton conducting membrane. There are a number of requirements to the membrane for fuel cell operation. The membrane must conduct hydrogen ions (protons) but not electrons. It must separate the gas or fuel flows on the anode and cathode. Finally, the membrane must be chemically stable and compatible with the structure of catalyst and gas diffusion layers, providing the lowest losses at the interface boundaries and not "poisoning" of catalysts over the range of operating temperatures and humidity [2].

Commercially available membranes, such as Nafion, demonstrate excellent chemical stability and high conductivity. However, their disadvantages are high cost and decrease of conductivity at low

relative humidity and high temperatures. So the main objective of this work is to develop highly thermal and mechanical stable proton conducting membranes for sustainable energy conversion and fuel cell applications with eco-friendly process [3].

We have developed a convenient method for the synthesis of composite membranes containing silicon dioxide blocks by the hydrolytic condensation of organosilicon precursors in the presence of organic polymers. The resulting membranes are characterized by high proton conductivity (1.35×10^{-2} to 4.2×10^{-2} S/cm), the activation energy of the proton transfer process of 24.5 kJ/mol and high ion exchange capacity (3.5 mg-eq/g) as well as thermal and mechanical stability.

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Fabrication of NiO/Ni Microfibers as Anode Material for Lithium-Ion Batteries with Enhanced Capacity and Rate Capability

An increase in the energy density and rate capability of lithium-ion batteries (LIB)s is required to meet the hard demands for hybrid electric vehicles and efficient energy storage. In commercial LIBs, graphite is used as anode. However, its capacity density is not enough for practical applications. So, there is an increasing interest in the possibility of using metal oxides instead of graphite, with the goal of reducing the electrode volume as well as achieving signifi-

cantly increased capacity [1]. NiO as anode material for LIBs has theoretical capacity of 718 mAh/g. In this work NiO electrode with nanostructured surface based on Ni microfibers was investigated.

For the synthesis of Ni microfibers, chemical method was used [2]. Ni/NiO electrode was prepared by oxidation of Ni fibers. For the electrode prepared via standard technique active material was mixed with binder and carbon superP. The

pressed electrodes and electrodes with fiber arrays were prepared without binder and conductive additives. The prepared electrodes were used as cathodes. Li foil was used as anode.

The surface of Ni fibers is roughened, and the diameter is around 1.2 microns. The rate capability and stability of the electrodes were studied. The maximal working currents were applied up to 10 C. The influence of the electrode preparation technique on the capacity fading and rate capability was studied. The specific capacity for fibers oxidized at 400 °C is more than 600 mAh/g. It was found that electrodes have demonstrated capacity of about 200 mAh/g at 10 C and after 200th cycle capacity retention up to 400 mAh/g.

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Transient Response of Electrochemical Power Sources as a Diagnostic Tool

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Electrochemical power sources (EPS) are one of the main energy sources for modern portable electronics. EPS has the requirements of high efficiency and power density as well as high short and long term reliability. Therefore the effective diagnostic tools are required. Diagnostic technique based on analysis of EPS transient responses caused by load variation has been proposed. The application of this approach to two different EPS types: lithium battery and hydrogen PEM fuel cell is considered. The selection of these two types is caused by the facts that lithium batteries are one of the most used and efficient modern power sources while PEM fuel cell (PEMFC) due to high efficiency and ecologically friendly utilisation is one of the most perspective elements. The advantage of the proposed technique is inexpensive measurement equipment and possibility to provide diagnostic during EPS operation.

It was found [1] that the transient response can be described with enough high accuracy by an instantaneous step and two exponential relaxation processes. The transient response is sensitive to the operating mode and technical state of the lithium batteries, for example, state of charge. Analysis of the experimental results for PEMFC shows that the parameter U_1 of the relaxation processes could be used to describe and study aging processes of PEMFC. Theoretical and experimental results prove that the transient response is a prospective diagnostic tool for EPS. The simplicity of hardware and software make it possible to embed the diagnostic tool into the EPS without significant increase in their cost.

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Influence of Crossover on the Columbic Efficiency of Vanadium Redox Flow Batteries

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The Vanadium Redox Flow Batteries (VRFB) are considered as one of the most promising technological pathways towards a large scale energy storage systems suitable for integration into the grids with distributed power generation [1]. The VRFB stores electrical energy in the chemical form of vanadium solutions converting it in the electrochemical cells and storing the electrolytes in two separated external tanks. Accordingly, the storage capacity and power rating of VRFB facilities can be scaled up independently. In addition, the VRFB has a very low self-discharge, long life time (more than 10 000 cycles and 20 years) and good tolerance to deep discharge [2].

One of the challenges rising up during operation of VRFB is the transfer of vanadium of ions across the membrane (or crossover) [3], that induces a build up of vanadium ions in one half-cell and the corresponding drop in the other half. Arisen imbalance in electrolytes will have influence on the battery capacity, which becomes limited by the half-cell with lowest vanadium concentration and volume [4], and consequently, the battery capacity drop will spring up. Induced capacity decay will, in turn, shorten the usable capacity in long-term operation, and therefore, needs to be detected and periodically corrected by electrolyte remixing [5]. Accordingly, to ensure a long operation of VRFB, it is indispensable to investigate capacity decay mechanism caused by crossover and to develop reliable capacity restoration methods.

The purpose of this work is to elucidate fundamental physical processes in the crossover and their influence on the cell columbic efficiency. The results of this work can be a useful tool for improvement of VRFB performance and the development of sustainable VRFB facilities.

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Evaluation of the Ir-Based Oxygen Evolution Catalysts for PEM Water Electrolyzers

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Among the various methods developed for hydrogen production from renewable energy sources, water electrolysis is considered as practical and flexible way. In particular, polymer electrolyte membrane (PEM) electrolysis offers a sustainable solution to produce hydrogen, which may be coupled with intermittent renewable energy sources (e.g. wind turbines and solar photovoltaic panels)[1].

Ir (IrO₂) is generally recognized as the state-of-the-art oxygen evolution reaction (OER) catalyst in PEM electrolysis as Ru (RuO₂) is much stronger and suffers from the instability (corrosion) in acid solutions [2,3]. In the case of components for more commercially available devices such as PEM fuel cells, one can find widely accepted testing protocols, but in case of PEM electrolyzers there is an absence of such protocols and procedures. Evaluation of the efficiency of OER catalysts is complicated by the lack of standardization both in the data measurement and reporting. Since the electrolyzer performance and lifetime significantly depend on the anode, the efforts addressed to easily evaluate and improve OER catalyst are required. A possible way to increasing the noble metal utilization is the deposition of Ir on a support material with high surface area.

The aim of this study is to evaluate the activity and stability as well as characterize the surface of different Ir-based OER catalysts (including Ir black, IrO₂ and Titania supported IrO₂) using electrochemical approaches. Moreover, to validate the procedure all evaluated catalysts were also studied in PEM WE electrolysis cell and their chemical and morphological ex-situ characterization were performed.

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Evaluation of Anion Exchange Membranes for Low Cost Alkaline-Based Water Electrolysis

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Hydrogen can be produced through several methods but currently the majority of hydrogen is produced from the steam reforming of natural gas, hydrocarbons and alcohols [1]. But water electrolysis has gained much attention, since it allows the relatively quick and convenient solution to produce hydrogen with high purity only from water and electricity [2].

Over the past few years, anion exchange membranes (AEMs) have been developed for electrochemical applications, mainly for use in alkaline fuel cells and they have been applied for water electrolysis in significant lesser degree [3]. AEM water electrolysis owns all conventional alkaline electrolysis technology advantages: the usage of inexpensive non-noble metal catalysts and stack materials (in contrast to the Nafion®-based membrane electrolysis) and easy handling due to the relatively low temperatures. Moreover, AEM electrolysis allows overcoming considerable disadvantage of conventional alkaline electrolysis like the usage of high concentrated and still low conductive alkaline

solutions (AEM could provide high conductivity at only 1M KOH solution or even pure water without the electrolyte carbonization process occurring).

In the presented study, several commercially available AEMs were studied using the nickel-based electrolysis cell with non-noble metal catalysts (NiFeCo and FeNiO₄) as cathode and anode catalyst respectively. Great attention was paid to the purity of generated hydrogen (intrinsic purity, without any auxiliary used) and the hydrogen yield. Also, the capability of tested membranes to operate only with pure water feeding without KOH was demonstrated.

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Novel Routes for the Processing of Thermoelectric Materials

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Thermoelectric materials generate a thermovoltage when exposed to a temperature gradient [1]. They are central components in thermoelectric generators, which allow to recuperate electric energy from waste heat leading to higher energy efficiency and lower emissions. Reduction of processing costs as well as opening up of novel applications coating- and film technologies [2] are in the focus of our research. Besides the thermoelectric properties of the compounds the mechanical properties of such layers and films play an important role for technical applications.

In this paper, a novel route for the preparation of thin films will be described and the influence of processing parameters will be addressed. For sample characterization physico-chemical measurements were used as well as the thermoelectric performance was characterized.

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Electrochemical Energy Storage

Battery Related Model Studies with Ionic Liquids

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Driven by automotive and portable applications, as well as by the demand for storing fluctuating electric energy from renewable energy sources, there is a need for improved batteries. Ionic liquids such as 1-butyl-1-methylpyrrolidinium bis-(trifluoromethane-sulfonyl) imide (BMP-TFSI) are promising candidates as electrolytes for future batteries due to their low vapor pressure and wide electrochemical potential window.

In this contribution, we present results of two model studies on the electrochemical properties of BMP-TFSI in simplified conditions/systems, aiming at a deeper understanding of the processes at the electrode | electrolyte interface.

In the first study, we explored the formation of the “solid electrolyte interphase” (SEI), which forms upon electrolyte reduction at the anode of lithium-ion batteries and hinders further solvent decomposition, using highly oriented pyrolytic graphite (HOPG) as model electrode. SEI formation in LiTFSI containing BMP-TFSI is characterized by cyclic voltammetry and the resulting elemental composition of the interphase is probed by XPS. We found that the SEI composition is very similar to the decomposition products formed upon vapor deposition of BMP-TFSI and Li.[1]

In the second case, the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER), which should occur during discharging and charging of Mg-air batteries, are studied on glassy carbon electrodes. Oxygen consumption and evolution are monitored by differential electrochemical mass spectrometry (DEMS), which allows us to determine the number of electrons transferred per O₂ molecule. This provides information on the selectivity of the ORR/OER with respect to the formation of superoxide or peroxide species, which is affected by the presence of Mg²⁺ ions.[2,3]



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Advanced Energy Storage: Challenges and Prospects



The development of advanced materials and technologies to efficiently convert and store energy directly into electricity is of urgent importance due to increasing energy demands of an ever growing world population and the growing need to diversify to renewable energy alternatives. However, tremendous scientific challenges remain before successful implementation of any number of competing energy technologies such as solar cells, fuel cells, and batteries can be adopted. The materials, interfaces and device architectures currently being explored are very challenging to interrogate by ensemble-averaging, bulk experimental methods since they do not exhibit long-range order or homogeneity, contain unique nano-morphological features and possess non-uniform chemical compositions

and defect chemistry. Additionally, these materials and interfaces are dynamically “reactive” and their performance degrades significantly during use which limits their cycle life and their ultimate commercialization prospects. This presentation will summarize a few materials design strategies for optimizing the performance of redox-active materials used in electrochemical energy storage applications. The development of high resolution spatially resolved tools for studying charge transfer processes at electrochemical interfaces will also be highlighted. Information obtained from these new tools enables the elucidation of complex electron and ion transfer mechanisms and degradation processes in existing and emerging materials considered for advanced electrochemical energy conversion and storage applications.



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Professor Stevenson received his Ph.D. in 1997 from the University of Utah. Subsequently, he held a postdoctoral appointment at Northwestern University (1997–2000); and a professorial appointment since 2000 at the University of Texas at Austin.

Stevenson’s research interests are aimed at elucidating and controlling chemistry at solid/liquid interfaces vital to many emerging energy storage and energy conversion technologies. To date he has published over 160 peer-reviewed publications, five patents, and six book chapters in this field.

At present, he is leading the development of a new graduate level university (Skolkovo Institute for Science and Technology) in Moscow, Russia where he is the Director of the Center for Electrochemical Energy Storage (CEE). The CEE conducts research that supports the energy industry in Russia and the world, and develops and demonstrates materials, devices and systems that provide the basis for innovative opportunities for advanced energy storage technologies.



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In-situ Monitoring the Formation of Luminescent Complexes: a New Spectroscopic Approach



The future of improved energy conversion, storage, harvesting and efficiency requires the development of new materials with novel and/or optimized properties. [1] This fact justifies the increased interest in a rational synthesis of such materials, by improving the understanding of their synthesis processes by means of the application of in-situ characterization techniques, seeking to overcome the lack of predictability of the product formation. This work presents the application of the new in-situ luminescence analysis of coordination sensors (ILACS) [2, 3] approach for monitoring the formation of a class of materials increasingly relevant for the production of organic light emitting diodes (OLEDs): the lanthanide (Ln) complexes. Here, different spectroscopic aspects as changes in the $4f \rightarrow 4f$ and $5d \rightarrow 4f$ electronic transition of Ln ions as well as on the energy-transfer behavior between them and changes in the ligand luminescence has been used for monitoring the formation of $[\text{Ln}(\text{L})(\text{NO}_3)_3]$ (Ln = Eu, Tb, Ce, Sm, L = 1,10-phenanthroline, 2,2'-bipyridine) in solution. [2-5] This way, not only the influence of reaction parameters such as reactant concentration and temperature have been determined, but also the formation of reaction intermediates has been revealed, confirmed by simultaneous measurements of synchrotron-based in-situ X-ray diffraction analysis. The new ILACS approach is highly advantageous in this field for being able to characterize besides crystalline compounds, also

amorphous materials and specimen in solution, also in conventional university laboratories, independent on large research facilities.

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Rechargeable Lithium-Ion System Based on Lithium-Vanadium(III) Phosphate and Lithium Titanate

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Lithium-ion batteries are the highest-capacity among commercialized rechargeable electrochemical systems. In their composition, lithium metal oxides of variable valency, mainly layered LiCoO_2 , are widely used as active materials of the cathode, and graphite is used as the material of the anode. The spread of the advantages of such batteries from devices for portable electronics to large-sized devices requires the use of materials which are not sensitive to possible overheating of the system and so safe in operation.

We consider issues related to the functioning of $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (LVP) and $\text{Li}_4\text{Ti}_5\text{O}_{12}$ (LTO) in one lithium-accumulating system as materials, of the positive and negative electrodes respectively. The functional materials that constitute the subject of the study were previously obtained by us [1-3].

The proposed electrochemical system $(-) \text{LTO} \mid 0.67 \text{ M LiClO}_4 \text{ in PC} + \text{DME} \mid \text{LVP} (+)$ includes materials of positive and negative electrodes which show the high electrochemical characteristics in cells with lithium counter electrodes. Testing the prototype with the proposed electrochemical system with the ratio of active substances LVP:LTO as 1:1 revealed its strong degradation in the first charge-discharge cycles. It has been shown experimentally that this degradation is associated with the loss of functional activity of lithium pentatitanate due to the accumulation of peroxides in the liquid electrolyte during the oxidation of 1,2-dimethoxyethane as the secondary process in the charging of the electrode containing LVP. The significant increase in the stability of the prototypes during cycling was observed when laying in them an excess of LVP corresponding to the elimination of the oxidation of V(IV) to V(V) as the final stage of the charge of this electrode material.

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In-situ Oil Upgrading: New Environmentally Friendly Technologies for Hydrocarbon Production

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Because of the exhaustion in traditional crude oil resource in the world, heavy oil reserves are attracting more and more attention. The growing in energy demand worldwide makes it essential to develop unconventional oil resources like heavy oil and bitumen [1-2]. However, heavy oil and bitumen are known for the high content of high-boiling molecules which gives the characteristic, such as high viscosity, high density/low API gravity, low yields of low-boiling fuel distillates, and high heteroatom content compared to light oil. The main challenge is to increase the efficiency of in-situ upgrading of heavy oils and bitumen, and thus increase the efficiency of hydrocarbons production and transportation due to decreasing viscosity, increasing API gravity and increasing light fractions of heavy oil. Steam injection is one of the main thermal methods for enhanced oil recovery (EOR) in the extraction of high-viscosity oils and natural bitumens. During the steam injection, the oil viscosity is decreased due to the increased temperature, which thus reduces the flow resistance and improves the oil mobility in the reservoirs. However, aquathermolysis occurs during the steam injection process, which usually leads to the coke formation and generates free radicals that initiate polymeri-

zation reactions and produce larger molecules that are more viscous than the heavy oil. Consequently, the quality of the crude oil will become worse. These problems can be solved by applying catalytic aquathermolysis technology.

Hydrothermal catalytic process in reservoir conditions (in-situ upgrading) has got remarkable attentions last years. In this study, the feasibility of the in-situ upgrading of heavy crude oil using steam and transition metal-based catalysts co-injection at different temperatures (250°C and 300°C) under high pressures was investigated in batch reactor.

The results were compared as the changes in the density/API gravity, viscosity, chemical composition (SARA analyses), FTIR-spectroscopy, elemental analysis of heavy crude oil before and after thermal treatment and gas-chromatography analysis of saturated and aromatic hydrocarbons before and after upgrading. In general we can conclude that, the content of resin and asphaltenes is decreased and the average molecular weight of heavy oil is reduced after hydrothermal catalytic processes. Whereas saturated and aromatic hydrocarbons content is increased as well as viscosity and API gravity changes were explored.

Ion Exchange in Zeolite 13X – Tuning of the Thermochemical Heat Storage Behavior

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The goal to exclusively use the regeneratively produced energy to meet the world's energy demand requires a continuous provision of energy. Green energy sources like solar or wind power are gaining more importance but are only discontinuously available. As a result of these aspects, the development of innovative storage concepts and materials is needed.

In comparison to other energy storage options, the method of sorptive heat storage is nearly loss-free and delivers high energy densities.[1] The heat storage is achieved by the ad- and desorption of small molecules, e.g. water. Zeolites have interesting properties,[2] which generate comparably high storage densities and feature high discharging temperatures over 100°C. However, for this class of materials, high charging temperatures (desorption of water) are needed.

In order to tune the materials properties like charging and discharging temperature, several concepts are available. The main principles to influence the zeolites properties are ion exchange and dealumination of aluminosilicate zeolite structures. Here zeolite X with faujasite structure type is an interesting candidate for modification.

Zeolite 13X and ion-exchanged zeolite 13X materials were investigated in terms of their storage properties. The starting material zeolite 13X contained Na⁺ ions, which were partial ex-

changed by Li⁺, Ca²⁺ and Mg²⁺ ions.[3] The ion exchange led to an increase of the water uptake ($g_{\text{water}}/g_{\text{zeolite,dry}}$) and the desorption energy. The exchange of Na⁺ ions by Li⁺ ions delivers more space for water molecules in the zeolite's pores. Mg²⁺ and Ca²⁺ ions possess higher hydration enthalpies. Therefore the ion exchange with such divalent ions led to a higher desorption energy and higher storage densities if appropriate desorption temperatures are applied.

Furthermore, the materials underwent a hydrothermal stress test to investigate their stability behavior during 20 charging cycles. Here we present the results for several modified zeolite X samples, which were synthesized and accurately characterized.

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Enhancing Na⁺ Extraction Limit through High Voltage Activation of the Nasicontype Na₄MnV(PO₄)₃ Cathode Materials

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The prospects of developing cheaper energy storage technologies along with the applicability of knowledge gained from designing lithium insertion electrodes motivate studies on Na-ion batteries.

Extensively investigated Na₃V₂(PO₄)₃ cathode material crystallizes in a rhombohedral NASICON-type structure, which consists of corner-shared transition metal octahedra and phosphate tetrahedra, providing a 3D-network of Na⁺ diffusion pathways. Upon (de)intercalation of 2 Na⁺ ions per formula unit, it delivers a highly reversible capacity of ~110 mAh/g, showing a biphasic voltage plateau at 3.4 V corresponding to the V⁴⁺/V³⁺ redox couple [1, 2].

In Na_{3+x}Mn_xV_{2-x}(PO₄)₃, the introduction of Mn(II) leads to the voltage increase and materials cost decrease compared with Na₃V₂(PO₄)₃ [3]. We found that in Na₄MnV(PO₄)₃ cycling within 2.5–3.8 V, potential range proceeds through both solid solution (Na₄MnV(PO₄)₃ ↔ Na₃MnV(PO₄)₃) and two-phase (Na₃MnV(PO₄)₃ ↔ Na₂MnV(PO₄)₃) processes. Also we observed an additional voltage plateau at ~3.8–4.0 V vs. Na/Na⁺ associated with

re-distribution of Na cations over available crystallographic positions and “unlocking” of the Na1 site, which previously was not considered being depopulated on Na⁺ extraction. Insertion of Na⁺-cations on discharge proceeds via a complete solid solution region. The experimentally observed reversible electrochemical capacity exceeds 110 mAh/g after raising cut-off voltage indicating extraction of more than 2 Na⁺ ions per formula unit.

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SCIENCE – BUSINESS – INNOVATION

Siemens AG

A programme section of the “German-Russian Week of the Young Researcher” was dedicated to the academia–industry partnership. Dr. Martin Gitsels, Vice president of Siemens Russia, gave an overview of the innovative technologies of Siemens putting the emphasis on the company’s cooperation with Russian universi-

ties and research institutes. Dr. Gitsels answered the questions of young researchers and revealed cooperation opportunities offered by Siemens to talented scientists. Participants of the Week presented their research projects and shared their experiences of leveraging research results into successful innovation.

SIEMENS



Dr Martin Gitsels

Vice-President and Director
of the Department of Corporate
Technologies of Siemens, Russia



SCIENCE ORGANISATIONS



GERMAN-RUSSIAN INSTITUTE FOR ADVANCED TECHNOLOGIES (GRIAT)



Dr Alsu Gilmetdinova
Director of GRIAT



Dr Sven Rost
Director of GRIAT

German-Russian Institute for Advanced Technologies (GRIAT) allows students to obtain dual degrees with partner universities from Germany.

GRIAT is a new global-scale project that is aimed at training highly-professional engineers in compliance with the most advanced German and Russian educational standards. Upon completion training a GRIAT graduate is conferred with two diplomas: KNRTU-KAI and a partner German University (Technical University of Ilmenau, Otto-von-Guericke University Magdeburg, Technical University Keiserslautern).

Mission The German-Russian Institute of Advanced Technologies (GRIAT) is a unique educational platform that unites German and Russian universities and companies, trains multilingual engineers with global engineering skills, encourages multinational research and development activities, and promotes cross-cultural understanding and friendship between Germany and Russia.

Our Goals and Objectives GRIAT's goal is to train highly skilled specialists in accordance with German standards of education within the walls of the leading engineering university in the Russian Federation – TU Kazan. Together with educational programs, students and faculty from both TU Kazan and German partner universities are working on joint research projects, collaborate with German and Russian engineering companies, exchange experiences and advanced industrial technologies through their educational projects in both countries.

As our goal is to have up to 1.000 students enrolled in our MSc courses by 2022, we are always ready to implement new MSc programs, to start new joint research projects or solve R&D projects given by the industry. Our current and new partners have the unique chance to join the process of training elite global engineers, who are much more competitive in the employment market due to the experiences they receive in the double degree program, thus enhance your reputation and status!

KAZAN NATIONAL RESEARCH TECHNICAL UNIVERSITY NAMED AFTER A.N. TUPOLEV

Kazan National Research Technical University named after A.N. Tupolev integrates education, science and industry. KNRTU-KAI named after A.N. Tupolev provides advanced training technologies and offers highly-competitive education with a strong base for conducting scientific research and making cutting-edge inventions. Outside of the formal activities the students are involved in a sports and cultural life full of exciting events.

A Brief History: It was established in 1932 as Kazan Aviation Institute (KAI). In 1973, it received the honor to bear the name of the famous aircraft designer A. N. Tupolev. In 1992, the institution received the status of University and was renamed the Tupolev Kazan State Technical University. In 2007, KAI among the 57 universities of Russia, became the winner of the national contest of innovative educational programs within the framework of the national project «Education».

Another milestone in the history of our university is the year 2010, when our university obtained the status of a National Research University and was renamed into Kazan National Research Technological University (KNRTU-KAI) in 2011. And, in 2014, the German-Russian Institute of Advanced Technologies (GRIAT) was opened.

Our Mission: To become the unique knowledge-based center with the most favorable environment for developing education, scientific research and innovations, for raising new gener-

ations of scientists, academics and engineers capable of putting and keeping the Russian industry in a world market orbit. Today KNRTU-KAI named after A.N. Tupolev is one of the largest technical universities of Russia.

Scientific Research: An educational process and scientific research are organized at KNRTU-KAI in a special style. It represents an organic combination of fundamental university education and science with their applied focus. The research infrastructure is being actively developed.

The training course on the Theory for Inventive Problem Solving is introduced into an educational process at KNRTU-KAI named after A.N. Tupolev. This is a scientific approach to inventive activities that makes it possible to extend the existing bounds in any areas of expertise and to achieve new results. The training is performed in compliance with CDIO-standards – a complex approach to engineering education: a set of general principles for creating training programs, their material and technical support, selecting and training lecturers.

KNRTU-KAI has a Certificate of Conformity to international standards in the field of educational services and scientific research ISO 9001:2000.

KNRTU-KAI is a member of the European Association of Universities and a participant of the Partnership of a European Group of Aeronautics and Space Universities PEGASUS.



Professor Dr Albert Gilmudinov
Rector of KNITU-KAI



Dr Tatiana Stanko
Vice-Rector of KNITU-KAI

DEUTSCHE FORSCHUNGSGEMEINSCHAFT (DFG)



Dr Wilma Rethage
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Deputy Head of Department
Scientific Affairs, DFG Bonn

The Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) is the biggest funding agency in Europe for the development of fundamental research with an annual budget of approximately 3 billion Euro. Its membership consists of German research universities, non-university research institutions, scientific associations and the Academies of Science and the Humanities. The DFG has expanded its presence in other research regions around the world with its seven liaison offices. The office Russia/CIS was opened in Moscow in 2003. Framework agreements on the co-funding of research projects and researcher mobility exist with the Russian Foundation for Basic Research (RFFI), the Russian Science Foundation (RSF).

How does the DFG promote young researchers? Creative and intelligent minds are the key to successful science and research. That is why the Deutsche Forschungsgemeinschaft places a special focus on promoting young researchers. We are committed to helping young talents pursue cutting-edge investigations in top-level settings and help them to become independent early on in their careers.

Flexible individual funding and customised excellence programmes give young researchers the opportunity to advance in their careers and undertake projects from all branches of science and the humanities. The DFG accepts funding proposals from researchers with a doctoral degree (PhD) who live and work in Germany or plan to do so in the future. PhD students are not supported individually, but can be, indirectly through the funding of programmes and projects.

Project-based doctoral and post-doctoral qualifications. For doctoral researchers, who like working in a team and value a well-designed framework, a **Research Training Group (RTG)** may be the right choice. It combines an ambitious research programme with target-oriented supervision and academic freedom to form an ideal environment

for a successful doctorate. Post-docs help design the research and qualification programmes of an existing RTG and explore new research topics for your future career.

Following completion of the doctorate there is the possibility to assume responsibility as an **investigator in an existent DFG-funded project**. This will give young researchers the opportunity to advance their qualifications and improve their career prospects by gaining experience and by building new networks.

The **Temporary Position** is a funding mechanism that provides young researchers with funding for a temporary post-doctoral position in conjunction with a proposal for a research grant. Researchers may select the scientific setting in Germany that they think will provide the best conditions for their project.

Excellence programmes. The Emmy Noether Programme is aimed at outstanding scientists and academics with at least two and no more than four years of post-doctoral research experience (or up to six years for licensed medical doctors). It allows young researchers to head their own independent junior research group that will work on a project for five or, in exceptional cases, six years. It offers a fast-track opportunity to qualify for a leading position in research.

For young researchers, who have all the qualifications for a professorship, the **Heisenberg Programme** may be the right option. This programme provides them with funding for up to five years so they can distinguish themselves further academically. There are two variations of the programme: the portable Heisenberg fellowship, which also allows one to go abroad for some time; and the Heisenberg professorship, which offers the prospect of acquiring a tenured position at a German university, provided the candidate receives a positive review.

GERMAN CENTRE FOR RESEARCH AND INNOVATION (DWIH)

The German Centres for Research and Innovation (DWIH) are a network of German research organisations, universities and research-based companies. In five cities around the world, the DWIH provide a joint platform for German innovation leaders, showcase the capabilities of German research and connect German researchers with local cooperation partners.

The core mission of the German Centre for Research and Innovation (DWIH) in Moscow is to represent German science, research and innovation in Russia. It provides information about the German research and innovation landscape and helps connect German and Russian researchers and decision makers in science and innovation. Through its activities the DWIH Moscow aims to foster deeper science and technology collaboration between Germany and Russia.

The activities of the DWIH Moscow are supported by German organisations with a leading role in science and innovation which are represented in Russia, such as the German Academic Exchange Service, the German Research Foundation, the Helmholtz Association, the Contact Office of the Ministry of Culture and Science of North Rhine-Westphalia, the Freie Universität Berlin, the German Historical Institute, the University Alliance Ruhr, Thuringia International, the Representation of the State of Lower Saxony in Moscow, the Alexander von Humboldt Foundation and the German Russian Chamber of Commerce.

Since 1st January 2017, the German Academic Exchange Service (DAAD) is responsible for the management of the German Centres for Research and Innovation (DWIH). At the local level, the individual DWIH design their activities in cooperation with their supporters in a local Advisory Board.



Dr Andreas Hoeschen
Director of the DWIH, Moscow



Mikhail Rusakov
Coordinator, DWIH Moscow



GERMAN ACADEMIC EXCHANGE SERVICE (DAAD)



Dr Andreas Hoeschen
Director of the DAAD Moscow



The German Academic Exchange Service (DAAD) is an association of German institutions of higher education (HEIs). Its budget is derived mainly from the German federal funding for various ministries, primarily the German Federal Foreign Office. It acts as an intermediary in the field of German foreign cultural policy and contributes to German science diplomacy. The DAAD supports the internationalisation of German universities, promotes the German language in academia abroad and as its core business facilitates academic exchange of students, doctoral candidates and researchers from and to Germany.

To strengthen German-Russian academic cooperation, the DAAD offers:

- grants and scholarships for Russian students, doctoral candidates and researchers for studying and research in Germany,
- grants and scholarships for German students, trainees, doctoral candidates and researchers for studying and research in Russia,
- funding for double degree programmes and academic exchange projects between German and Russian HEIs,
- support for German lecturers and other German teaching staff at Russian HEIs,
- information, advice and networking opportunities for collaboration with German HEIs.

THE HELMHOLTZ ASSOCIATION

HELMHOLTZ SPITZENFORSCHUNG FÜR GROSSE HERAUSFORDERUNGEN

The Helmholtz Association was created in 1995 to formalize existing relationships between several globally-renowned independent research centers. The Helmholtz Association distributes core funding from the German Federal Ministry of Education and Research (BMBF) to its, now, 18 autonomous research centers and evaluates their effectiveness against the highest international standards. The Association's work follows in the tradition of its namesake, the natural scientist Hermann von Helmholtz (1821–1894).

The Helmholtz Association pursues the long-term research goals of the state and society, including basic research, in scientific autonomy. To do this, the Helmholtz Association conducts top-level research to identify and explore the major challenges facing society, science and the economy. Helmholtz Association scientists focus on researching the highly-complex systems which determine human life and the environment.

The Helmholtz Association brings together 18 scientific-technical and biological-medical research centers, a high-performance infrastructure and modern research management. With more than 39,000 employees and an annual budget of over € 4.5 billion, the Helmholtz Association is Germany's largest scientific organization. Its work is divided into six research fields: Energy, Earth & Environment, Health, Aeronautics, Space and Transport, Matter, and Key Technologies.

Within the six research fields, Helmholtz scientists cooperate with each other and with external partners – working across disciplines, organizations and national borders. The Helmholtz Association uses this research to create an effective basis for shaping the future. An excellent research

infrastructure – in some cases with unique major scientific facilities and instrumentation – clearly demonstrates the strength which has made the Helmholtz Association a much sought-after research partner. Each year, several thousand visiting scientists from all around the world use the research opportunities which the Helmholtz Centers offer. The Association acts as a core focal point for worldwide research project – whether in the observation and study of the global climate or in the field of basic research in physics. The Helmholtz Association aims to be an active and driving force in establishing the research area worldwide. This is why Helmholtz opened branch offices in Brussels, Moscow and Beijing. In the autumn of 2018 the Helmholtz Association is scheduled to open an office in Tel Aviv/Israel.

The Helmholtz Association chose Russia to be one of its key strategic partners to jointly face the challenges of the future through scientific cooperation. Partners in Germany looking for specific information about Russia and Russian seeking contacts in Germany have an excellent starting point in identifying the right people for their special interests. The transfer of new technologies and the exchange of promising young research talent hold great potential for the future development of both Germany and Russia. The Moscow Office represents the interests of Helmholtz Association as a whole in Russia. It serves both Helmholtz scientists and Russian researchers interested in mutual cooperation. Its main tasks are to provide help for scientific partners to establish contacts, to promote joint projects and to foster the exchange of scientists, with the goal of helping initiate and establish new strategic networks of scientific excellence between Russia and Germany.



Dr Elena Eremenko

Head of Helmholtz, Moscow Office



THE ALEXANDER VON HUMBOLDT FOUNDATION



Professor Dr Vladimir Tishkov

Ambassador Scientist
of Humboldt Foundation
Moscow State University,
Faculty of Chemistry

The Alexander von Humboldt Foundation promotes academic co-operation between excellent scientists and scholars from Germany and abroad. AvH research fellowships and research awards allow scientists to come to Germany to work on a research project they have chosen for themselves, together with a host and a collaborative partner. As an intermediary organization for German foreign cultural and educational policy, AvH promotes international cultural dialogue and academic exchange.

What is important to us? Only one thing is important to becoming a member of the Humboldt Family: your own excellent performance. There are no quotas, neither for individual countries nor for particular academic disciplines. AvH selection committees comprise of academics from all fields of specialisation and they make independent decisions based solely on the applicant's academic record. So in this case people are supported, not specific projects. After all, even in times of increased teamwork, it is the individual's ability and dedication that are decisive for academic success.

Roots of the AvH: Alexander von Humboldt was a discoverer and cosmopolitan. He was a fighter for the freedom of research, a humanist and a patron of excellent academic talent. Shortly after his death, the Alexander von Humboldt Foundation for Nature Research and Travel was established in 1860. Today's Alexander von Humboldt Foundation was established by the Federal Republic of Germany on 10 December 1953. With Humboldt as a mod-

el, the Foundation maintains an international network of academic co-operation and trust. It links more than 25,000 Humboldtians throughout the world together, including 49 Nobel Laureates. The Foundation is funded by the Federal Foreign Office, the Federal Ministry of Education and Research, the Federal Ministry for Economic Co-operation and Development, the Federal Ministry for the Environment, Nature Conservation and Nuclear Safety as well as a number of national and international partners.

Become a Humboldtian: Whether you are a young post-doctoral researcher at the beginning of your academic career, an experienced established academic, or even a world authority within your discipline – our research fellowships and research awards offer you sponsorship specifically tailored to you and your career situation.

Key Sponsorship Programmes:

- Research Fellowships for post-doctoral researchers and for experienced researchers (up to 24 months of stay in Germany).
- Awards (Sofja Kovalevskaja Award, Friedrich Wilhelm Bessel Research Award, Humboldt Research Award, Alexander von Humboldt Professorship and others).
- German Chancellor Fellowships to prospective leaders from the USA, the Russian Federation and China who have shown outstanding potentials for leadership in their careers so far, for representatives of all professions and disciplines, giving special preference to humanities, law, social science and economics.

BERLIN – AT THE EDGE OF BASIC AND APPLIED RESEARCH



The 8th Week of the Young Researcher stands in an already long line of conferences dedicated to bringing together young academics from Russia and Germany. Fostering careers in science by developing professional networks is one of the key elements of Freie Universität Berlin's career path model. Career development of young researchers is a cornerstone of the "International Network University" concept, successful in the German Excellence Initiative in 2007 and 2012. It is therefore no surprise that Freie Universität Berlin has been present at all prior weeks and has actively taken part with about half a dozen keynote speakers and more than a dozen doctoral students and young scientists. Interdisciplinary topics such as "Men and Energy", "Global History", "Discrete Geometry", and "Computational Biology and Biomedicine" are core research fields of Freie Universität, and the conference weeks have therefore been actively supported by the Moscow liaison office from the very outset.

The three main formats of the Week – opening session, keynote lectures by experienced German and Russian scientists, and young researchers giving short presentation or participating in poster sessions – are open to all interested specialists and even students of the hosting institution. Early career researchers are actively involved in the conference and get a first impression on how conferences conducted entirely in English "feel." Especially in light of the rising demand to integrate oneself internationally into the scientific community, the weeks of the young researcher offer

a great possibility to gain first experience. Many opportunities – not only during the lectures and scientific sessions, but also during excursions, evening receptions, and coffee breaks – are available for socializing and networking.

This year's conference location at German-Russian Institute of Advanced Technologies (GRIAT) allowed young researchers and students to join for one or another session, which they actively did throughout the week. Already for the second time, Kazan was an excellent place to organize the week and the GRIAT as an outstanding initiative of German-Russian cooperation provided an excellent platform.

The role of Freie Universität Berlin's liaison offices, in seven countries around the globe, is not only to attract highly talented young researchers to the exciting scientific environment in Berlin. It also supports scientists in Berlin who are interested in foreign experience to learn more about the respective regions, to motivate them to pursue a research stay abroad, and to connect with (young) colleagues, e.g., in Russia. High-level conferences, like the 2018 Week on Chemical Energy Storage and Conversion are ideal for fostering networks between the next generations of scientists at the edge of basic and applied research. Although it is still a major challenge to plan scientific careers, Freie Universität Berlin offers excellent opportunities for career advancement, including structured doctorate programs with its professional development program and postdoc fellowships offered within the Dahlem Research School.



Tobias Stüdemann

Liaison Office of Freie Universität
Berlin in Moscow



CONTACT OFFICE OF THE MINISTRY OF CULTURE AND SCIENCE OF THE FEDERAL STATE OF NORTH RHINE-WESTPHALIA



Ekaterina Karpushenkova

Contact Office of the Ministry
of Culture and Science
of the Federal State
of North Rhine-Westphalia

Ministry of Culture and Science of the Federal State of North Rhine-Westphalia has been operating a contact office in Moscow on interuniversity and research cooperation since 2005.

North Rhine-Westphalia (capital city Duesseldorf) is the leading German State not only in economy but also in the field of science and research where innovative ideas become reality. The densest scientific region in Europe with 72 universities and more than 50 non-university research institutions offers the best conditions to find answers to the major social challenges and to open up the markets of tomorrow. For North Rhine-Westphalia these are primarily the markets for new materials, mechanical and plant engineering and production technology, health, information and communications, mobility and logistics, energy and environmental economics, life sciences and the media and creative industries. They have a particularly high potential for the economy and employment and thus have a high priority for the economic development of the state. These topics are also reflected in the content orientation of universities. The close cooperation between an innovative, industrial economy and outstanding research enables a quick transfer of ideas into practice.

The Russian Federation is one of the key countries for North Rhine-Westphalia in the field of international scientific cooperation.

The contact office in Moscow conducts together with its German partner – center of innovation and technique ZENIT GmbH the project “Cooperation axis North Rhine-Westphalia – the Russian Federation”. The requests from relevant universities and research organizations from both sides in the field of science and development of cooperation are being processed and supported in the establishment of bilateral contacts in the Russian Federation and in the state of North Rhine-Westphalia.

The tasks of the contact office of the Ministry of Culture and Science of the Federal State of North Rhine-Westphalia in Moscow are:

- The first contact person for universities and research institutes from Russia and North Rhine-Westphalia;
- Marketing and publicity to promote the state of North Rhine-Westphalia as a center for innovation and research;
- Representation of North Rhine-Westphalia at conferences, exhibitions, seminars, specialized forums and negotiations;
- Bilateral support in establishing contacts with universities and research institutes;
- Accompanying delegations from North Rhine-Westphalia and Russia in cooperation with ZENIT GmbH;
- Providing of information on support programs and initial support for joint projects.

RUSSIAN SCIENCE FOUNDATION (RSF)



With an annual budget of about US\$ 370 million (fiscal year 2018), RSF is the premier research funder in Russia providing sufficient financial support for the cutting-edge research projects in all branches of frontier science, including humanities. Scientists and scholars of any nationality and in any discipline can apply to the RSF for a grant to undertake research at the frontiers of knowledge.

Since 2014, about 40,000 project proposals have been submitted to the RSF, of which, to date, some 3,000 have been selected for funding, representing an investment in 2018 of US\$ 308 million and 30,000 researchers, including 18,000 young scientists, from 541 host organizations nationwide. Over 10,000 articles acknowledging RSF support were published in international peer reviewed journals in 2017. At least half of each research team funded by the RSF are the young scientists aged under 39, which contributes to the training of a new generation of excellent researchers in Russia.

Through peer-reviewed competitions the most promising research projects, the best scientists are funded to perform their research in Russia. The recipients of the RSF grants enjoy a stable long-term prospective for their research with all necessary financial support provided for their significant research contribution to the global science as well as to the Russian economy and society.

In a multi-layered decision-making process, each proposal is evaluated by 2 to 5 external reviewers from Russia and abroad exclusively according to

scientific criteria; on the basis of this expert review, it is assessed by the members of an expert panel, and the final decision is made by an interdisciplinary expert council consisting of 63 members that are regularly rotated by research community on the basis of the voting process.

A new ambitious presidential programme to support early-career researchers was launched by the RSF in the spring 2017. This programme resulted during 2017–2018 in awards for 1007 young scientists under the age of 33 (20,000–30,000 euros annually for 2 years with a special relocation bonus) and for 552 youth research groups (40,000–80,000 euros annually for 3–5 years). These youth-support programmes have become regular grant opportunity provided by the RSF on a yearly basis.

The RSF actively encourages international research cooperation. The Foundation participates in a number of bilateral funding schemes that provide assistance to the best Russian researchers to participate in collaborative research projects with researchers abroad based on the principles of excellence, parity funding, credible independent peer-review and mutual trust.

The RSF secured a diversified portfolio of the bilateral collaborations with funders from Germany (DFG, Helmholtz Association), France (ANR), Belgium (FWO), Austria (FWF), Japan (MAFF), India (DST) and Taiwan (MOST). As a result in 2018 70 international collaborative projects were co-funded by RSF in amount of US\$ 6,7 million.



Dr Alexander Khlunov
General Director of the RSF



Dmitry Sergeev
Senior Specialist,
Division of Project and Programs



LIST OF PARTICIPANTS

TITLE	LAST NAME	FIRST NAME	POSTION / INSTITUTION
Ms	ABRAMKINA	Darya	PhD student, Heat, Gas Supply and Ventilation Systems Moscow State University of Civil Engineering
Dr	ABDEL MAGEED	Ali	Research Fellow, Institute of Surface Chemistry and Catalysis University of Ulm
Dr	ANDRONESCU	Corina	Postdoctoral Researcher, Analytical Chemistry Center for Electrochemical Sciences Ruhr – University Bochum
Prof. Dr	ANTIPOV	Evgeny	Corresponding Member of the Russian Academy of Sciences; Professor, Electrochemistry Department, Faculty of Chemistry Moscow State University
Prof. Dr	BEHM	Rolf Jürgen	Director, Institute of Surface Chemistry and Catalyse University of Ulm
Prof. Dr	BEHRENS	Malte	Professor, Center for Nanointegration Duisburg-Essen; DFG-Collaborative Research Center Transregio "Heterogeneous Oxidation Catalysis in the Liquid Phase"; University of Duisburg-Essen
Prof. Dr	BENSCH	Wolfgang	Speaker of the DFG Review Board "Chemical Solid State and Surface Research"; Professor at the Institute for Inorganic Chemistry, University of Kiel
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Prof. Dr	GILMUTDINOV	Albert	Rector, Kazan National Research Technical University named after A.N. Tupolev – KAI
Dr	GITSELS	Martin	Russia Vice President, Siemens AG

TITLE	LAST NAME	FIRST NAME	POSTION / INSTITUTION
Dr	GOEPEL	Michael	Post-doctoral Researcher, Institute of Chemical Technology University of Leipzig
Dr	HEUMANN	Saskia	Group Leader, Max Planck Institute for Chemical Energy Conversion Mühlheim
Dr	HOESCHEN	Andreas	Head of DAAD Office Moscow, Director of DWIH Moscow
Ms	ILINA	Julia	DFG Office Russia/CIS, Moscow
Ms	KARPUSHENKOVA	Ekaterina	Representative of the Ministry of Culture and Science of the German State of North Rhine-Westphalia in Russia
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Mr	KRUGLOV	Denis	Project Assistant, DWIH Office Moscow
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Dr	LEVIN	Oleg	Associate Professor, Electrochemistry, Saint Petersburg State University
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Dr	LUNKENBEIN	Thomas	Group Leader, Department of Inorganic Chemistry Fritz Haber Institute of the Max Planck Society Berlin
Dr	MAKISHA	Nikolay	Director, Water Supply and Waste Water Treatment Moscow State University of Civil Engineering
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Dr	MOROZOV	Mikhail	Associate Professor, Kazan National Research Technical University named after A.N. Tupolev – KAI
Mr	MÜLLER	Christian	Deputy Secretary General, German Academic Exchange Service Bonn
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Mr	PUGACH	Mikhail	PhD student, Energy Systems Center Skolkovo Institute of Science and Technology
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Ms	PUSHKAREVA	Irina	Research fellow, National Research Center "Kurchatov Institute"; Moscow Power Engineering Institute (National Research University)

TITLE	LAST NAME	FIRST NAME	POSTION / INSTITUTION
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Ms	SAVOSTINA	Anna	Project Coordination and Public Relations, DWIH Office Moscow
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Dr	SCHNAIDT	Johannes	Research Associate, Electrochemical Energy Storage Helmholtz Institute Ulm
Mr	SERGEEV	Dmitry	Senior Specialist, Division of Project and Programs Russian Science Foundation, Moscow
Ms	SHEVEREVA	Svetlana	Deputy Head, Division of International Bilateral Cooperation International Relations Department Russian Foundation for Basic Research, Moscow
Mr	SHIPILOV	Aleksey	Project Coordination and Public Relations, Helmholtz Association of German Research Centres, Moscow Office
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Mr	STÜDEMANN	Tobias	Head of the Liaison Office of Freie Universität Berlin in Moscow
Prof. Dr	TISHKOV	Vladimir	Ambassador Scientist of Humboldt Foundation, Professor, Faculty of Chemistry Moscow State University
Mr	USHAKOV	Arseni	Assistant Professor, Institute of Chemistry Saratov State University
Dr.	VARFOLOMEEV	Mikhail	Faculty of Chemistry Kazan Federal University
Ms	WILLKOMM	Juliane	PhD student, Department of Industrial Chemistry Otto von Guericke University of Magdeburg
Mr	ZAKHARKIN	Maxim	PhD student, Center for Electrochemical Energy Storage Skolkovo Institute of Science and Technology, Moscow; Moscow State University



PROGRAMME

September 10, Monday

- 20:30 **WELCOME PARTY**
- Words of Welcome to the participants of the week by
- Dr Andreas Hoeschen, DWH/DAAD Moscow
 - Dr Wilma Rethage, DFG Russia/CIS
 - Dr Tatiana Stanko, Vice-Rector of KNITU-KAI
- Introduction of the participants

September 11, Tuesday

- 10:00 Registration of Participants
- 10:30 **OFFICIAL OPENING OF THE WEEK**
- with welcome addresses by
- Professor Dr Albert Gilmutdinov, Rector of KNITU-KAI
 - Michael Dobis, Head of the Division for Science and Research, German Embassy Moscow
 - Christian Müller, Deputy Secretary General of the DAAD
 - Dr Johanna Kowol-Santen, Deputy Head of Department Scientific Affairs
- 11:30–12:15 **OPENING LECTURE**
- “Inorganic Materials for the Catalytic Generation and Chemical Storage of Hydrogen”
- Professor Dr Malte Behrens**
- University of Duisburg-Essen
- Discussion – (12:15–12:30)
- 12:30 Conference Group Photo
- 13:00 Lunch Break
- 14:00 **PRESENTATION OF GRIAT**
- Dr Alsu Gilmetdinova, Director of GRIAT
- Dr Sven Rost, Director of GRIAT
- 14:30 **LECTURE**
- “Alkali and Transition Metal Fluoride-Phosphates as Perspective Cathode materials for Metal-Ion Batteries”
- Professor Dr Evgeny Antipov**
- Lomonosov Moscow State University
- Discussion –
- 15:00 **LECTURE**
- “Anode Materials for Sodium Ion Batteries”
- Professor Dr Wolfgang Bensch**
- University of Kiel
- Discussion –
- 15:30 Coffee Break

16:00–18:00 **SHORT LECTURES OF YOUNG RESEARCHERS**

(20 min)

"Battery Related Model Studies with Ionic Liquids"

Dr Johannes Schnaidt

University of Ulm

"Novel Fluoride-Phosphate based High-Energy Cathode Materials for the Next Generation of Rechargeable Batteries"

Dr Stanislav Fedotov

Skoltech Moscow / Moscow State University

"Enhancing Na⁺ Extraction Limit Through High Voltage Activation of the Nasicon-Type Na₄MnV(PO₄)₃ Cathode Materials"

Maxim Zakharkin

Skoltech, Moscow / Moscow State University

"Rechargeable Lithium-Ion System Based on Lithium-Vanadium(III) Phosphate and Lithium Titanate"

Dr Arseny Ushakov

Saratov State University

"Influence of Crossover on the Columbic Efficiency of Vanadium Redox Flow Batteries"

Mikhail Pugach

Skoltech, Moscow

Chair: Evgeny Antipov

September 12, Wednesday

09:00 **LECTURE**

"Multi-electron Redox Electrode Materials for Li- and Na-Ion Batteries"

Dr Nina Kosova

Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk

– Discussion –

09:30 **LECTURE**

"Organometallic Electrode Materials for New Generation of Batteries"

Dr Oleg Levin

St. Petersburg State University

– Discussion –

10:00 Coffee Break

10:30 **LECTURE**

"Advanced Energy Storage: Challenges and Prospects"

Professor Dr Keith Stevenson

Skoltech, Moscow

– Discussion –

11:00 **SHORT LECTURES OF YOUNG RESEARCHERS**

(20 min)

"In-situ Luminescence Analysis of Coordination Sensors (ILACS): Looking Inside Chemical Reactions"

Dr Huayna Terraschke

University of Kiel

"Rare-Earth Ions as Local Probes in Hydrides and Mixed Anionic Hydrides"

Dr Nathalie Kunkel

Technical University of Munich

11:00 (20 min)	<p>"Sustainable hydrogen production via ammonia decomposition over bi-metallic iron catalysts: Room Promotional effect of gallium and cobalt"</p> <p>Dr Klaus Friedel Ortega University of Duisburg-Essen</p> <p>Chair: Wolfgang Bensch</p>
12:00	Lunch Break
13:00	<p>LECTURE</p> <p>"Fabrication of NiO/Ni Microfibers as Anode Material for Lithium-ion Batteries with Enhanced Capacity and Rate Capability"</p> <p>Dr Mikhail Morozov KNITU-KAI, Kazan</p> <p>– Discussion –</p>
13:30 (20 min)	<p>SHORT LECTURES OF YOUNG RESEARCHERS</p> <p>"Cell Design Aspects in lab scale electrocatalytic CO₂ reduction experiments"</p> <p>Jonas Geisler University of Jena</p> <p>"Influence of Temperature and Electrolyte Concentration on the OER Catalytic Activity of NiFe LDH"</p> <p>Dr Corina Andronesco Ruhr University of Bochum</p> <p>"Carbon Based Electrodes – A Black Prospect for a Bright Future"</p> <p>Dr Saskia Heumann Max Planck Institute for Chemical Energy Conversion</p> <p>"A Local View on Cu/ZnO/Al₂O₃ Catalysts for Methanol Synthesis"</p> <p>Dr Thomas Lunkenbein Fritz Haber Institute of the Max Planck Society, Berlin</p> <p>"Sunlight Driven CO₂ Valorization via Photocatalysis and Heterogeneously Catalyzed Glycolic Acid Upgrading"</p> <p>Dr Michael Goepel University of Leipzig</p> <p>"Production and Use of Biogas as an Alternative Source of Energy"</p> <p>Dr Nikolay Makisha Moscow State University of Civil Engineering</p> <p>Chair: Malte Behrens</p>
15:30	<p>PRESENTATIONS OF THE MEMBER ORGANISATIONS</p> <p>of the DWIH (Deutsches Wissenschafts- und Innovationshaus / German Centre for Research and Innovation)</p> <p>Dr Andreas Hoeschen, Director</p>
16:00	<p>SCIENCE CAFÉ</p> <p>Presentation of the Funding Programmes of German and Russian Funding and Research Organisations (Alexander von Humboldt Foundation, DAAD, DFG, Freie Universität Berlin, Helmholtz Association, Ministry of Culture and Science of the German State of North Rhine-Westphalia in Russia, Russian Science Foundation, Russian Foundation for Basic Research, Thuringia International in Russia)</p>

- 17:00
(20 min) **SHORT LECTURES OF YOUNG RESEARCHERS**
- "Design of Catalysts for Carbon Dioxide Valorization under Mild Conditions"
Ruslan Lukin
Kazan Federal University
- "Evaluation of Anion Exchange Membranes for Low Cost Alkaline-based Water Electrolysis"
Irina Pushkareva
Moscow Power Engineering Institute (National Research University)
- "Evaluation of the Ir-based Oxygen Evolution Catalysts for PEM Water Electrolyzers"
Artem Pushkarev
Moscow Power Engineering Institute (National Research University)
- Chair: Keith Stevenson**
- 19:30 Evening Reception by the DWIH-Moscow (German Centre for Research and Innovation)

September 13, Thursday

- 09:00 **LECTURE**
- "Electrochemical Noises of PEM Fuel Cells and Their Diagnostic Properties"
Associate Professor Dr Evgenii Denisov
KNITU-KAI, Kazan
– Discussion –
- 09:30 **SCIENCE – BUSINESS – INNOVATION**
- "Industries-University Cooperation – The Siemens' Approach"
Dr Martin Gitsels
Russia Vice President, Siemens AG
- 10:00 **LECTURE**
- "Novel Routes for Processing of Thermoelectric Materials"
Professor Dr Franziska Scheffler
University of Magdeburg
– Discussion –
- 10:30 Coffee Break
- 11:00 **SHORT LECTURES OF YOUNG RESEARCHES**
- "Controlling Activity and Selectivity for CO₂ Methanation on Highly Active Ru/TiO₂ Catalysts"
Dr Ali Abdel-Mageed
University of Ulm
- "Micro-macro-porous Composite Materials for Sorptive Heat Storage and Cooling"
Dr Alexandra Lieb
University of Magdeburg
- "Determination of Water Adsorption Kinetics and Adsorption Enthalpies – Experimental Setup and Challenges"
Jacob Eggebrecht
University of Magdeburg
- "Ion Exchange in Zeolite 13X – Tuning of the Thermochemical Heat Storage Behavior"
Juliane Willkomm and Dr Alexandra Lieb
University of Magdeburg

11:00	<p>"Solar Chimney with Heat-Accumulator Layer"</p> <p>Darya Abramkina</p> <p>Moscow State University of Civil Engineering</p> <p>Chair: Franziska Scheffler</p>
12:40	Lunch Break
13:30	<p>Lecture</p> <p>"Electrode – Electrolyte Interactions in Batteries: Model Studies from a Surface Science Perspective"</p> <p>Professor Dr Jürgen Behm</p> <p>University of Ulm</p> <p>– Discussion –</p>
14:00	<p>Lecture</p> <p>"Underground Petroleum Refining: New Technologies for Hydrocarbon Production"</p> <p>Dr Mikhail Varfolomeev</p> <p>Kazan Federal University</p> <p>– Discussion –</p>
14:30	Coffee Break
15:00 (20 min)	<p>Short Lectures of Young Researchers</p> <p>"Ionothermal Carbons for Energy-Related Applications"</p> <p>Dr Tim-Patrick Fellingner</p> <p>Technical University of Munich</p> <p>"Development of New Proton Conductive Membranes for PEM Fuel Cells"</p> <p>Sergey Maksimenko</p> <p>Irkutsk National Research Technical University</p> <p>"Transient Response of Electrochemical Power Sources as a Diagnostic Tool"</p> <p>Timur Nikishin and Guzel Timergalina</p> <p>KNITU-KAI, Kazan</p> <p>Chair: Mikhail Varfolomeev</p>
16:00	Closing Remarks

September 14, Friday

15:00-17:00 Falling Walls Lab at Kazan Federal University

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