The Department of Inorganic Chemistry - Functional Materials at the University of Vienna invites you to attend the KIT-50 symposium on the occasion of the 50th birthday of Prof. Freddy Kleitz

KIT-50

An Honorary Symposium for Professor Freddy Kleitz's 50th Birthday Celebration

Time: *June 3rd 2022;* 10.15 - 16.40

Location: Faculty of Chemistry, University of Vienna, Währinger Straße 42 A-1090 Wien; Joseph Loschmidt Hörsaal / Großer Hörsaal 2 (HS2)

Program:

10.15-10.40	Opening Session	
10.40-11.10	PD Dr. Claudia Weidenthaler	“For a chemist's curiosity: in situ characterization of inorganic solids”
11.10-11.40	Dr. Wolfgang Schmidt	“A walk with nanoporous materials - what have we learned?”
11.40-12.10	Prof. Dr. Mika Lindén	“20+ years of common interest in mesoporous materials – From mechanism of formation to application”
12.10-13.20	Break	
13.20-13.50	Priv.-Doz. Dr. Harun Tüysüz	“Mesostructured Cobalt-based Oxides for Water Electrolysis”
13.50-14.20	Rémy Guillet-Nicolas, PhD	“Adsorption in small pore zeolites: Impact of composition and pore network”
14.20-14.50	Prof. David Grosso, PhD	“Sol-gel metal oxide functional coatings and patterns elaborated through dip-coating and Nano-Imprint Lithography”
14.50-15.30	Coffee Break	
15.30-16.00	Mike Janicke, PhD	ERDE: a method for high-resolution NMR using the Earth’s Magnetic Field”
16.00-16.30	Prof. Dr. Matthias Thommes	“Adsorption and phase behaviour of pure fluids in hierarchically organized nanoporous materials over a wide range of temperatures and pressures”
16.30-16.40	Closing remarks	

Univ.-Prof. Dr. Freddy Kleitz received his MSc in Chemistry in 1996 at the Université Louis Pasteur - University of Strasbourg in France, under the supervision of Dr. Michel Pfeffer. After, he moved to Brazil and worked under the direction of Prof. Jairton Dupont as research assistant. In 1998, he joined the group of Ferdi Schüth in the Department of Heterogeneous Catalysis at the Max-Planck-Institut für Kohlenforschung in Germany and competed his PhD studies in inorganic chemistry there in 2002. Soon after, he joined the Korea Advanced Institute of Science and Technology (KAIST) in South Korea to work with Professor Ryong Ryoo as a postdoctoral researcher. He returned to the Max-Planck-Institut as a Max-Planck fellow by the end of 2003. In 2005, Prof. Kleitz moved to Canada, where he took an Assistant Professor position in the Department of Chemistry at Université Laval in Quebec City. In 2010, he was promoted to the rank of Associate Professor, and he became a full professor in 2014. In 2016, Prof. Freddy Kleitz was appointed as a University Professor at the Faculty of Chemistry at the University of Vienna, where he is now the Head of the Department of Inorganic Chemistry – functional materials. In 2011-2012, he was a visiting professor in the ARC Centre for Functional Nanomaterials (Australia Institute for Bioengineering and Nanotechnology, University of Queensland, Brisbane). Since 2014, he has been a guest Professor at the China University of Petroleum in Qingdao, China.

Professor Freddy Kleitz has published almost 200 refereed research articles, communications, and book chapters and which have been cited more than 11,000 times (H index = 54; Web of Science). He is frequently invited to be a speaker at academic and industry institutions around the world (more than 60 invited lectures in academia/industry and more than 50 oral presentations at international conferences including 20 invited talks). Since the beginning of his carrier he has been awarded more than 30 research grants, honors, and scholarships. He has supervised more than 80 graduate and undergraduate students and senior scientists. Prof. Kleitz has been an advisory committee member or advisory board member of several international organizations and journals in the fields of inorganic chemistry and materials science. He is currently the President of Chemical-Physical Society (Chemisch-Physikalische Gesellschaft; CPG) based in Vienna. He is also an associate-editor for the journals of Microporous and Mesoporous Materials and Materials Today Sustainability (Elsevier).

His main research activities concentrate on the development of functional materials exhibiting well-defined pores below 100 nm. These high-surface-area materials exhibit proper particle morphologies and incorporate functional groups for selective sorption and separation, heterogeneous catalysis, and biomedical applications. The research emphasizes the design of hybrid materials by selective positioning of guest species in specific sites inside inorganic matrices. In addition to the practical technological aspects, his research aims to provide fundamental insights into host-guest interactions within nanopores, adsorption processes, confinement effects, interfacial interactions, and transport phenomena at the nanoscale.

Invited Speakers:

1. *PD Dr. Claudia Weidenthaler - Research Group Leader Heterogeneous Catalysis, Powder Diffraction and Surface Spectroscopy, Max-Planck Institut für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany; weidenthaler@mpi-muelheim.mpg.de*

For a chemist's curiosity: in situ characterization of inorganic solids

If we want to understand the structure-property relationships of functional materials in detail, a comprehensive characterization of the corresponding materials under reaction conditions is essential. Diffraction, scattering, and spectroscopy are often used to investigate structural changes induced by a reaction. However, as the experience has shown, the examination of a material before and after reactions is often insufficient to understand its behaviour during the specific reaction. Today, in situ investigations under non-ambient conditions, such as temperature increase, can be considered standard methods. One step further, operando studies under working conditions enable the correlation of structural changes with performance data. Different possibilities will be discussed on how one could get insights into various chemical and structural processes. The focus of the presentation is on energy-relevant materials, mostly inorganic catalysts.

Image source: https://www.kofo.mpg.de/person/101007/2552

2. Dr. Wolfgang Schmidt - Research Group Leader, Functional Materials, Heterogeneous Catalysis, Max-Planck Institut für Kohlenforschung, 45470 Mülheim an der Ruhr, Germany; schmidt@mpi-muelheim.mpg.de

A walk with nanoporous materials - what have we learned?

About 35 years ago, when I started working on nanoporous materials, a certain knowledge existed on some materials, others were not known at all at that time. I found it interesting to ponder about the development of the field over the years and realized that many of the participants contributed significantly to the field. Shortly before the millennium, a young Frenchman popped up at our department with whom I had the pleasure to walk along our scientific way for quite some time. I will talk about our stroll and about the pleasure we had in investigating the materials we had at hand and on other developments that were made along our way, as reflected from the perspective of knowledge that we have achieved by now. Has there been progress or are we still poking along in misty fog?

Image source: https://www.kofo.mpg.de/person/101006

3. Prof. Dr. Mika Lindén - Head of Institute for Inorganic Chemistry II, Universität Ulm, 89081 Ulm, Germany; mika.linden@uni-ulm.de

20+ years of common interest in mesoporous materials – From mechanism of formation to application

It is a pleasure and an honour for me to have been given the chance to contribute to the 50 year-celebrations of Freddy´s. During the last more than 20 years our common interest in mesoporous materials research has led to some 10 common papers, and I want to take the opportunity to summarize some of these results. Having met for the first time in Frankfurt in the group of Ferdi Schüth´s, and being part of the same EU funded project focusing on the mechanistic aspects of the formation of surfactant-templated mesoporous silicas, our paths crossed again in Mülheim/Ruhr in 2003. Our initial collaborations focused on silicas synthesized in the presence of cationic small-molecular surfactants, and these studies were extended towards corresponding materials synthesized in the presence of non-ionic, polymeric surfactants. While the early studies were focused on wet systems, the focus shifted gradually to the investigation of structural and surface-chemical properties of the dry solids. After Freddy moved to Canada we still stayed in personal contact, but the practical scientific collaborations kicked off again more actively after Freddy moved back to Europe and Vienna. During the last decade we have both been interested in using mesoporous silica materials for theranostics, and our latest common papers are focused on understanding the interrelation between surface functionalization and serum protein adsorption. I am extremely thankful for having had the opportunity to collaborate with Freddy, and even more for the close friendship we have developed over the years. All the best Freddy for your birthday, and I look forward to what the next decade will bring.

Image source: https://www.uni-ulm.de/nawi/nawi-anorg2/institut/mitarbeiter/mika-linden/

4. Priv.-Doz. Dr. Harun Tüysüz - *Head of Research Group of Heterogeneous Catalysis and Sustainable Energy, 45470 Mülheim an der Ruhr, Germany; tueysuez@kofo.mpg.de*

Mesostructured Cobalt-based Oxides for Water Electrolysis

Ordered mesoporous materials offers many fascinating physicochemical properties and can be implemented as toolbox to study structure-activity correlations towards development of more effective electrocatalyst [1]. Water electrolysis is a very promising process to split water into green H_2 and O_2 gases by using sustainable electricity. Among both half-reactions of the water electrolysis, oxygen evolution reaction (OER) is thermodynamically more challenging due to multiple electron transfer and oxygen-oxygen formation. Despite a great process in the research field, the commercial OER catalysts are still mainly based on iridium and ruthenium, which are not appropriate for large-scale applications owing to their limited resources and costs. Consequently, there is a need for development of more active and sustainable OER electrocatalysts, preferably based on abundant first-row transition metals [2]. The lecture will cover some of our progress about design and development of mesostructured cobalt oxides and cobalt-based mixed oxides for the OER [3, 4]. The impact of the incorporation of silver species into ordered mesoporous cobalt oxide, distortion of crystal and electronic structures, and phase segregation of ordered mesoporous cobalt iron oxide nanowires on their OER activity in alkaline electrolyte will be elaborated, as summarized in below Figure.

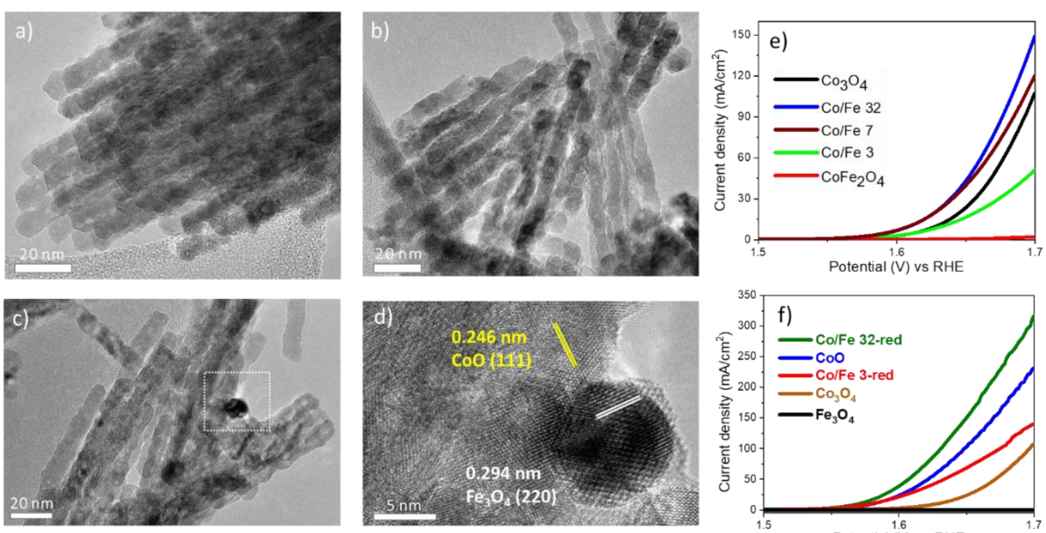

Figure 1 TEM images of replicated Co_3O_4 nanowires (a) and selected cobalt iron oxide replica with Co/Fe ratio of 32 (b), TEM and HR-TEM images of replicated cobalt iron oxide after reduction (c

and d), and linear sweep voltammogram curves of a series of replicated cobalt oxide nanowires before (e) and after reduction (f).

References

[1] M. Yu, G. H Moon, R. Castillo, S. DeBeer, W. Weidenthaler, H. Tüysüz, *Angew. Chem. Int. Ed.* **2020,** 59, 16544

[2] M. Yu, E. Budiyanto, H. Tüysüz, *Angew. Chem. Int. Ed.* **2022**, *61,* e202103824

[3] E. Budiyanto, M. Yu, M. Chen, S. DeBeer, O. Rüdiger, H. Tüysüz, *ACS App. Energy Mater* **2020**, 3, 8583

[4] E. Budiyanto, s. Salamon, Y. Wang, H. Wende, H. Tüysüz, *JACS Au* **2022**, *2, 697*

Image source: https://www.uni-due.de/sfbtrr247/people/tuysuz.php

*5. **Rémy Guillet-Nicolas, PhD** - Researcher CNRS, Laboratory of Catalysis and Spectrochemistry (LCS), ENSICAEN, Normandy University, 14050 Caen, France; remy.guillet-nicolas@ensicaen.fr*

Adsorption in small pore zeolites: Impact of composition and pore network

With the ongoing energetic transition, a lot of focus is being set on the purification and transportation of gas mixtures containing high added value molecules such as CO_2, N_2, H_2, CH_4, etc. However, all technologies associated with the obtention of relevant high energy density products are, so far, outrageously energy and investment intensive if not applied at a very large scale. Therefore, direct processes for gas separation, storage, and transportation, economically applicable at a small and medium scale would be of great interest. Despite existing technical barriers, adsorbed gas technologies (AG) appear as a promising solution. Indeed, physisorption at moderate pressures/temperatures in highly porous materials remain one of the cheapest and easiest option. The key point for this technology to succeed lies in the development of better adsorbent. In this way, thanks to their outstanding physico-chemical properties, small pore zeolites continue to be among the best candidates. However, while much knowledge has been accumulated so far in their design and modifications, the relationship between the synthesis parameters, the resulting pore topologies/ architectures and adsorption capacities needs to be further investigated and improved. The main aim of present the work is thus to evaluate the effect of zeolite pore architecture and composition on adsorption capacities of small gases and selectivity of their mixture's separations.

Image source: https://www.mintova.cnrs.fr/remy-guillet-nicolas/

6. Prof. David Grosso, PhD - Institut Matériaux Microélectronique et Nanosciences de Provence, (IM2NP) - UMR CNRS 7334, NOVA Team, Aix-Marseille Université, Faculté des Sciences de Saint Jérôme, Université de Toulon, 13397 Marseille Cedex 20, France; David.grosso@im2np.fr

Sol-gel metal oxide functional coatings and patterns elaborated through dip-coating and Nano-Imprint Lithography

Complex hierarchical nano structured (hybrid) coatings can be achieved when combining chemical advanced bottom-up strategies, such as self-assembly and sol-gel chemistry, together with liquid solution processing. This communication reports first on the recent implementations of the dip-coating process, including controlled atmosphere, capillary deposition, thickness gradient, deposition from supernatant, angle dependence deposition, and single side deposition. Besides, in most applications, sol-gel coatings interact with the ambient atmosphere and physical-chemical properties may be altered through temperature and humidity variation or adsorption of volatiles species present in the surrounding medium. Such phenomena are difficult to assess and it will be demonstrated that ellipsometry is not only a technique adapted to deduce optical constant and physical thickness of optical layers, but is also highly appropriated to the determination of adsorption/desorption mechanisms. Finally, many microfabrication tools can be used to further process the coating and obtained controlled patterns, amongst which soft-nano imprint lithography (Soft-NIL) has proven to be simple to apply to the as-prepared xerogel. This approach will be discussed in terms of adjustment of critical processing parameters and applications in controlled wetting, photonics and gas detection will be presented.

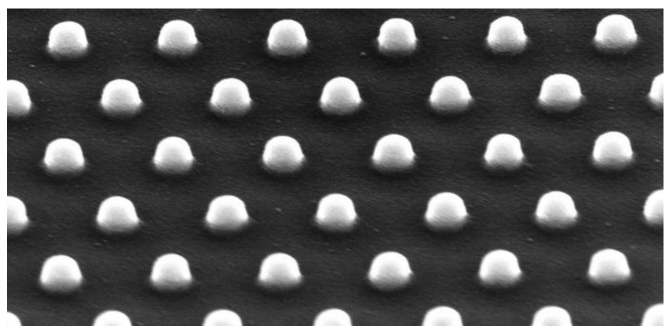

Image source: https://www.im2np.fr/fr/david-grosso

7. Mike Janicke, PhD – *Nuclear and Radiation Studies Board, The National Academy of Sciences, Washington DC, USA*
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ERDE: a method for high-resolution NMR using the Earth's Magnetic Field

Originally a character in Richard Wagner's epic Opera, *Der Ring des Nibelungen,* Erda (Jörð, goddess of the earth and mother of Thor) advises Wotan that there exists irrevocable destruction and death to anyone who tries to possess the Ring. While this was a danger in Norse legends, other more worldly threats exist today that are challenging to deter, detect, and defend. The focus of this presentation is chemical threats. While Erda gave the warning on how to protect the world, herein I will describe our team's successful efforts to use *die Erde* in a means of protection, to recognize dangerous and clandestine substances like Sarin, VX, or Novichok. A program I was able to develop at Los Alamos National Lab focused on pinpointing methodologies to identify these chemical agents using new technology that were small and portable, not cost prohibitive, defensible in forensic applications, and safe for operators. By pulling together a team with specialties in chemistry, physics, and engineering, Nuclear Magnetic Resonance spectroscopy (NMR) methods using low magnetic fields (Millitesla) and the earth's magnetic field (Microtesla) were developed to demonstrate the feasibility of magnetic resonance methods. The system assembled and recently patented is a home-built spectrometer using the Earth's magnetic field for NMR spectroscopy. Aptly named ERDE, Earth-field Resonance Detection and Evaluation device, at this ultra-low field the well-known chemical shift information is loss, but precise J coupled spectrum can be measured. These spectra could serve as unique fingerprints for chemical agents with better fidelity than commercial high field or benchtop spectrometers.

BIOGRAPHY: Michael Janicke graduated from Rice University and the Ph.D. program at the University of California Santa Barbara with degrees in chemical engineering. Following his studies, he was awarded Alexander von Humboldt and Max Planck Society postdoctoral fellowships at the Max Planck Institute for Carbon Research before starting his research career at Los Alamos National Lab. He also notes that he learned some French in Mülheim an der Ruhr. His expertise is in heterogeneous catalysis, microreactor systems, porous materials, and NMR. He has published nearly 50 articles with over 4,500 citations in peer-reviewed literature. Michael is currently a senior program officer at the National Academy of Sciences and the study director in a project to address the adequacy of US strategies to prevent, counter, and respond to nuclear terrorism and assisting to examine the use of analytical methods to assess the risks of nuclear terrorism and nuclear war. The job involves a lot of paperwork and reading.

Image source: https://www.researchgate.net/profile/Michael-Janicke-2

8. *Prof. Dr. Matthias Thommes – Head of Department of Chemical and Biological Engineering (CBI), Head of Institute for Separation Science & Technology, Friedrich-Alexander-University, Erlangen-Nürnberg, 91058 Erlangen, Germany; matthias.thommes@fau.de*

Adsorption and phase behaviour of pure fluids in hierarchically organized nanoporous materials over a wide range of temperatures and pressures

Peter Leicht, Simon Eder and Matthias Thommes*

Adsorption of CO_2 in porous materials plays an important role in different applications. Among them are CO2-capture from flue gas and other industrial waste streams as well as upgrading natural gas and biogas for pipeline transport. Understanding the fundamental adsorption mechanisms and phase behaviour of the adsorptive in the pore system can help to identify critical adsorbent properties that influence process performance. Within this context, the adsorption and phase behaviour of mainly CO_2 but also CH_4 and other alkanes/alkenes in hierarchically structured nanoporous materials (e.g, hierarchical zeolites) and ordered mesoporous materials was studied over a wide range of temperatures (subcritical and supercritical) and pressures using volumetric and gravimetric techniques. An accurate textural characterization (e.g., pore volume/size distribution, pore network characteristics) of the adsorbent materials was obtained by advanced gas adsorption studies coupled with the application of methods such as non-local density functional theory (NLDFT) and molecular simulation. This allows for an *in-depth* correlation of the CO_2 and CH_4 adsorption behaviour with the surface- and pore characteristics. Our results lead to a better understanding of how confined geometry effects contribute to the adsorption and phase behaviour of CO_2 and CH_4 in hierarchically structured nanoporous materials. These insights allow one to explore important aspects related to applications such as gas storage and filtration/purification processes.

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