

3rd CENIDE Conference 2023



UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

3rd CENIDE Conference 2023

May 02-04, 2023

Kardinal-Schulte-Haus, Overather Str. 51, 51429 Bergisch Gladbach https://tagen.erzbistum-koeln.de/ksh





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Conference Program

	Tuesday, May 2	Wednesday, May 3	Thursday, May 4
08:00–08:30		Breakfast	Breakfast
08:30–09:00			
09:00–09:30	Arrival, Registration and	Invited Keynote Talk:	Impulse Presentations
09:30–10:00	Collee	Robert Schlogi	New Topics $B(3)$, $C(6+7)$
10:00–10:30	Welcome and CENIDE Overview Talk	Coffee Break	Coffee Break
10:30–11:00	Postdoc Session I	Postdoc Session II	Workshops B (3), C (6+7)
11:00–11:30			
11:30–12:00			
12:00–12:30	Lunch	Lunch	
12:30–13:00			Workshops Summary C Closing Remarks
13:00–13:30	Impulse Presentations	Walking and Talking	Lunch
13:30–14:00	New Topics A (1-2)		
14:00–14:30	Workshops New Topics A		Departure
14:30–15:00	(1-2)	Impulse Presentations New	
15:00–15:30		Торіся в (4+5), С (8)	
15:30–16:00		Workshops New Topics B	
16:00–16:30	Workshops Summary A	Coffee Break	
16:30–17:00	Coffee Break		
17:00–17:30	Film Picture a Scientist		
17:30–18:00		Workshops Summary B	
18:00–18:30		Invited Keynote Talk:	
18:30–19:00		Katharina Kohse-Höinghaus	
19:00–19:30	Poster Session I	Poster Session II	
19:30–20:00	with Dinner		
20:00–20:30			
20:30–21:00			
21:00	Get-Together with Drinks	Get-Together with Drinks	



Tuesday, May 02, 2023

- 09:00–10:00 Arrival and Registration and Coffee
- 10:00–10:30 *Welcome and CENIDE Overview Talk* Heiko Wende

Postdoc Session I

Chair: Heiko Wende

- 10:30–10:45 Structure and Stability of Artificial Oxygen Carriers Studied by X-ray Scattering on the Nanoscale Martin Schroer
- 10:45–11:00 Electrocatalytic Activity of Fe-based Materials for the Oxygen Evolution Reaction: Influence of Surface Arrangement Ricardo Martínez-Hincarpié
- 11:00–11:15 Pilot-Scale Preparation of Nickel-Cobalt Based Anode Materials for Alkaline Water Electrolysis Vineetha Vinayakumar – **CENIDE Early Career Fellow**
- 11:15–11:30 Mechanism and Effect of Gold Nanorod Uptake in Immune Cells Tista Roy Chaudhuri
- 11:30-11:45 Secondary Ion and Neutral Mass Spectrometry for the Nano-Scale Lars Breuer
- 11:45–12:00 Gas-Phase Synthesis: Graphene and Soot Evolution, Coated Nanomaterials, and New Templating Methods Claudia-F. Lopez-Camara – **CENIDE Early Career Fellow**

12:00-13:00 Lunch

Impulse Presentations and Workshops: New Topics A (1-2) Chair: Sebastian Schlücker

- 13:00–13:20 *A.1 Magnetism & Non-equilibrium Dynamics* Andrea Eschenlohr, Heiko Wende
- 13:20–13:40 A.2 Quantum Technologies Gerd Bacher
- 14:00–16:00 Workshops New Topics A (1-2)
- 16:00–16:30 Summary and Discussions A.1+A.2 in Plenum

16:30–17:00 Coffee Break



Film Picture a Scientist Chair: Doris Segets

17:00–18:30 Film Picture a Scientist

18:30–19:00 Open Discussion

- 19:00–21:00 Poster Session I with Flying Dinner
- 21:00 Get-Together with Drinks

Wednesday, May 03, 2023

08:00-09:00 Breakfast

Invited Key Note Talk I Chair: Marika Schleberger	
09:00–10:00	Hydrogen – How much? When? Robert Schlögl
10:00–10:30	Coffee Break
Postdoc Ses	sion II
Chair: Marika	Schleberger
10:30–10:45	Optical Properties of Two-Dimensional Antiferromagnetic NiPS3 Monolayers Encapsulated by Hexagonal Boron Nitride Pradeep Kodimana Ramakrishnan – CENIDE Early Career Fellow
10:45–11:00	Large Eddy Simulations of Nanoparticle Synthesis in Spray Flames Seung-Jin Baik – CENIDE Early Career Fellow
11:00–11:15	Hydrogen Production via Dark Fermentation by Bacteria Colonies on Porous PDMS-Scaffolds Miriana Vadalá
11:15–11:30	Porous Polymeric Multi-Composites with a Tailored Nickel Microenvironment as Catalytic Flow-Through Membrane Reactors for Efficient p-Nitrophenol Degradation Lukas Fischer
11:30-11:45	Investigating the Inception Process of Carbonaceous Particles: from Flames to Shock-Tube Can Shao
11:45–12:00	Characterization of Particle Dynamics and Orientational Phenomena in Soft, Magnetic Hybrid Materials Joachim Landers



12:00-13:00 Lunch

13:00–14:30 Walking and Talking

Impulse Presentations and Workshops: New Topics B (3-5) Chair: Christof Schulz		
14:30–14:50	C.8 Magnetism & Catalysis Rossitza Pentcheva, Stephan Schulz, Heiko Wende	
14:50–15:10	B.4 Electrochemical Systems Christof Schulz, Doris Segets	
15:10–15:30	<i>B.5 Nano-Bio-Medicine</i> Sven Brandau, Sebastian Schlücker	
15:30–17:30	Workshops New Topics B (3-5) + Coffee Break	
17:30–18:00	Summary and Discussions B.3+B.4+B.5 in Plenum	
Invited Key N Chair: Christo	lote Talk II f Schulz	
18:00–19:00	Thoughts on Excellence Katharina Kohse-Höinghaus	
19:00-21:00	Poster Session II with Flying Dinner	

21:00 Get-Together with Drinks

Thursday, May 04, 2023

08:00-09:00 Breakfast

Impulse Presentations and Workshops: New Topics C (6-8) Chair: Nils Weimann		
09:00–09:20	C.6 Additive Manufacturing Michael Giese, Stefan Kleszczynski	
09:20–09:40	<i>C.7 Hydrogen</i> Harry Hoster, Moritz Pilaski	
09:40–10:00	<i>B.3 Artificial Intelligence</i> Karin Everschor-Sitte, Heiko Wende	
10:00-10:30	Coffee Break	



10:30–12:30 Workshops New Topics C (6-8)

12:30–13:00 Summary and Discussions C.6+C.7+C.8 in Plenum +Closing Remarks

13:00-14:00 Lunch

14:00–14:30 Departure

Workshops:

#	Торіс	Persons in Charge
A.1	Magnetism & Non-equilibrium Dynamics	Andrea Eschenlohr, Heiko Wende
A.2	Quantum Technologies	Gerd Bacher
B.3	Artificial Intelligence	Karin Everschor-Sitte, Heiko Wende
B.4	Electrochemical Systems	Christof Schulz, Doris Segets
B.5	Nano-Bio-Medicine	Sven Brandau, Sebastian Schlücker
C.6	Additive Manufacturing	Michael Giese, Stefan Kleszczynski
C.7	Hydrogen	Harry Hoster, Moritz Pilaski
C.8	Magnetism & Catalysis	Rossitza Pentcheva, Stephan Schulz, Heiko Wende



Talks

Postdoc Session I

1: Structure and Stability of Artificial Oxygen Carriers Studied by Xray Scattering on the Nanoscale

Martin A. Schroer¹, Ozan Kamaran², Jan-Eric Sydow², Fabian Nocke³, Katja B. Ferenz^{2, 4}

¹ Nanoparticle Process Technology (NPPT), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

² Institute of Physiology, University Hospital Essen / University of Duisburg-Essen, Hufelandstr. 55, 45122 Essen, Germany

³ Institute of Physiological Chemistry, University Hospital Essen / University of Duisburg-Essen, Hufelandstr. 55, 45122 Essen, Germany

⁴ CENIDE (Center for Nanointegration Duisburg-Essen), University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany

E-Mail: martin.schroer@uni-due.de

Red blood cell concentrates (RBC) are an indispensable tool in various clinical scenarios; however, the available quantity is already highly limited, which will become an even more severe problem in the future. To overcome these peculiarities and limitations of RBCs, we developed albumin-derived perfluorocarbon-based artificial oxygen carriers (A-AOCs), that are comprised of a perfluorodecalin (PFD) microemulsion core and an albumin shell, and have already successfully supplied oxygen in extra-corporally perfused hearts and various animal models [1]. The structure and stability of A-AOCs is sensitive to changes of the carrier solution, so we need to learn more about the structure and structural changes on the nanoscale. Conventional characterization techniques lack the spatial resolution (*e.g.* light scattering) or need dried and thus non-physiological samples (*e.g.* SEM, TEM), and thus yield limited information on A-AOC structure in solution. We therefore used (ultra-)small angle X-ray scattering (USAXS), which does not have such limitations and allows studying also especially dense, opaque suspensions.

In our contribution, we present recent results of (U)SAXS measurements on A-AOCs covering a wide, clinical-relevant concentration and temperature range. We investigate A-AOCs from different synthesis approaches, using ultra-sound [2] and microfluidizing techniques, which reveal different sizes and stabilities. Based on these findings, it is now possible to optimize the synthesis parameters, in order to yield stabile A-AOCs of wanted size and dispersity.

This study therefore shows the huge potential of X-ray scattering for the study of pharmaceutical and medical-relevant samples [3], with direct implications for the development of new formulations

- [1] J. Jägers, A. Wrobeln, K.B. Ferenz, *Pflugers. Arch.* **473**, 139 (2021).
- [2] A. Wrobeln, J. Laudien, C. Gross-Heitfeld, J. Linders, C. Mayer, B. Wilde, T. Knoll, D. Naglav, M. Kirsch, K.B. Ferenz, *Eur. J. Pharm. Biopharm.* **115**, 52 (2017).
- [3] S.S. Nogueira, A. Schlegel, K. Maxeiner, B. Weber, M. Barz, M.A. Schroer, C.E. Blanchet, D.I. Svergun, S. Ramishetti, D. Peer, P. Langguth, U. Sahin, H.Haas, *ACS Appl. Nano Mater.* **3**, 1063 (2020).



2: Electrocatalytic activity of Fe-based Materials for the Oxygen Evolution Reaction: Influence of Surface Arrangement

Ricardo Martínez-Hincapié¹, Viktor Čolić^{1, 2}

¹ Electrochemistry for Energy Conversion, Max-Planck-Institute for Chemical Energy Conversion ² Center for Nanointegration Duisburg-Essen (CENIDE)

E-Mail: ricardo.martinez-hincapie@cec.mpg.de

The conversion of renewable energy into storable fuels or chemicals is fundamental to the meeting of the net-zero CO_2 emissions objective by 2050. However, the high overpotential of the oxygen evolution reaction (OER) and the poor stability of electrocatalysts at industrial-level currents remain a challenge [1]. Using earth-abundant metals as electrocatalysts for the OER is an appealing strategy due to the low cost and acceptable activity and stability. In particular, Febased materials offer the possibility for the development of active, stable, and cost-effective electrocatalysts for the OER in alkaline media.

The influence of structure, composition, or crystalline phase on different Fe-based electrodes for the OER had been studied using different electrochemical techniques. Different fabrication procedures such as additive manufacturing [2], flame spray synthesis [3], or pulse laser ablation [4] allow us to have a wide range of Fe-based materials with a well-defined structure/composition/phase. The materials have been extensively characterized by physicochemical methods (XPS, Raman, XRD, ICP) and their electrocatalytic activity evaluates following careful procedures in order to obtain reliable results. The results show that the activity of Fe-rich electrodes is poor. However, if Fe is alloyed with other materials or its surface structure or crystallinity degree is modified, it results in a more active material. This information could guide to synthesize more active and stable water-splitting materials.

- [1] I. Katsounaros, S. Cherevko, A.R. Zeradjanin, K.J.J. Mayrhofer, Oxygen Electrochemistry as a Cornerstone for Sustainable Energy Conversion, Angewandte Chemie International Edition, 53 (2014) 102-121.
- [2] J. Wegner, R. Martínez-Hincapié, V. Čolić, S. Kleszczynski, Additively Manufactured Iron-Based Bulk Metallic Glass Composite Electrocatalysts: Effect of Microstructural States on the Oxygen Evolution Reaction Activity, Advanced Materials Interfaces, n/a (2023) 2202499.
- [3] S. Angel, F. Schneider, S. Apazeller, W. Kaziur-Cegla, T.C. Schmidt, C. Schulz, H. Wiggers, Spray-flame synthesis of LaMO3 (M = Mn, Fe, Co) perovskite nanomaterials: Effect of spray droplet size and esterification on particle size distribution, Proceedings of the Combustion Institute, 38 (2021) 1279-1287.
- [4] J. Johny, Y. Li, M. Kamp, O. Prymak, S.-X. Liang, T. Krekeler, M. Ritter, L. Kienle, C. Rehbock, S. Barcikowski, S. Reichenberger, Laser-generated high entropy metallic glass nanoparticles as bifunctional electrocatalysts, Nano Research, 15 (2022) 4807-4819.





3: Pilot-scale preparation of Nickel-Cobalt based anode materials for alkaline water electrolysis

<u>Vineetha Vinayakumar</u>¹, Adarsha Kumara Adagalale Jinadath¹, Mohit Chatwani¹, Timo Wagner², Christian Marcks³, Nicolas Wöhrl^{2,4}, Anna K. Mechler³, Doris Segets^{1,4}

¹ Institute for Energy and Materials Processes–Particle Science and Technology (EMPI–PST), University of Duisburg–Essen (UDE), Duisburg, Germany;

² Faculty of Physics, University of Duisburg–Essen (UDE), Duisburg, Germany;

³ Electrochemical Reaction Engineering, RWTH Aachen University, Aachen,

Germany;

⁴ Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen (UDE), Duisburg, Germany;

Email: vineetha.vinayakumar@uni-due.de

Renewable energy has become more popular in recent years as traditional sources of energy have depleted. The production of hydrogen and oxygen from water electrolysis is becoming increasingly desirable and is currently experiencing rapid advancements. Nevertheless, it remains challenging to upscale stable and high-efficiency anodes for alkaline water electrolysis into a pilot-scale synthesis in order to establish direct property-performance correlations in industrial settings₁.

In this study, we aim to close this gap by introducing a defined way of characterizing inks and electrode layers using complementary techniques that enable coherence along the design process. In the first step, Ni- and Co-based commercial micro powders were characterized for their size and composition using transmission electron microscopy and energy-dispersive Xray spectroscopy. Using analytical centrifugation and therefrom derived Hansen parameter calculations₂, ink formulations and their recipes were appropriately optimized. Selected dispersions were then coated on Ni plates through ultrasonic spray deposition to obtain the respective electrodes. In addition, the effect of surface plasma treatment was investigated to induce surface modifications and enhance electrode film stability. To make electrode features quantifiable, a framework was developed to analyze the electrode's surface features using atomic force microscopy. After such in-depth assessment of structural properties, the generated electrodes were tested for their functionality as anode catalysts for alkaline water electrolysis. This enabled to correlate their physicochemical properties with electrochemical activity and stability. The developed methodology now enables us to evaluate the entire system at different stages and to feed back the acquired knowledge for further enhancement of the characteristics of the electrode. This is particularly important to expand lab-scale developments towards pilot-scale processing relevant for industrial applications.

- [1] Kang, Z., Nano Energy 47, 434-441 (2018)
- [2] Bapat, Shalmali., ACS Applied Nano Materials 3.8, 7384-7391 (2020)



4: Mechanism and effect of gold nanorod uptake in immune cells.

<u>Tista Roy Chaudhuri ^{1,2}</u>, Ronja Schirrmann ², Sayantan De ³, Rebeka Bosnjakovic ², Helene Giesler ¹, Michelle Hechler ¹, Barbara Sacca ³, Sebastian Schlücker ¹, and Sven Brandau ²

¹ Department of Physical Chemistry, University of Duisburg-Essen ² Department of Otorhinolaryngology, University Hospital Essen ³ Department of Bio-nanotechnology, University of Duisburg-Essen

E-Mail: Tista.Chaudhuri@ext.uk-essen.de

The tumor microenvironment of solid cancers harbors tumor-promoting immune cells [1], and eliminating these cells using gold nanorods (AuNR) coupled with heat-ablating photothermal therapy (PTT) may activate anti-tumor immunity. The goal of our study was to establish the immunological effects of AuNR uptake by phagocytic neutrophils (PMNs) and non-phagocytic T cells.

AuNR uptake by whole blood showed that the AuNRs were preferentially phagocytosed by PMNs and dendritic cells (DC) significantly more than by macrophages and other non-phagocytic immune cells. The AuNRs were up-taken non-specifically by phagocytic PMNs, and they accumulated over time within late endosomal and lysosomal vesicles; this induced ER stress and evoked an acute pro-inflammatory response via. LOX-1 induction, significantly higher expression of CD11b, IL8 secretion and ROS production [2]. We also discovered that the non-specific uptake of AuNRs by PMNs was size- and shape-dependent. Increasing the size of the AuNRs (15nm to 60nm) resulted in enhanced uptake by PMNs; additionally, rod-shaped particles showed significantly higher uptake compared to gold nanospheres. In contrast, non-phagocytic T cells showed significantly lower AuNR-uptake, which increased significantly upon targeting T cell surface antigen CD3 with monoclonal antibodies (mAbs); anti-CD3-AuNR conjugates bound to T cells with greater affinity compared to non-specific mAb-conjugated controls, and induced selective cytotoxicity by heat generated via PTT. These findings suggest that the AuNRs can be targeted to T cells via mAb-dependent uptake. In contrast, phagocytic monocytes and PMNs showed non-specific uptake of the AuNRs, including of non-specific IgG-conjugated AuNRs, and thereby mediated widespread cytotoxicity with PTT. Given that AuNR uptake by PMNs is shapeand size-dependent, non-specific target-independent uptake must be overcome by modifying surface charge and coat of the AuNRs. Finally, AuNR-loaded PMNs were able to migrate into tumor spheroids grown in vitro as a 3D co-culture, and induced tumor cytotoxicity when exposed to radiation by PTT.

Therefore, the AuNR+PTT system can be potentially utilized to actively target T cells and passively target pro-tumor PMNs in the tumor microenvironment to evoke anti-tumor immunity. Additionally, manipulating surface properties and enhancing biocompatibility of AuNRs may overcome non-specific uptake by PMNs.

- [1] Si Y, Merz SF, Jansen P, et al. *Sci. Immunol.* 4, 40 (2019).
- [2] Schirrmann R, Erkelenz M, Lamers K, et al. ACS Nano. 16, 7 (2021).





5: Secondary Ion and Neutral Mass Spectrometry for the Nano-Scale

Lars Breuer¹

¹ Fakultät für Physik, Universität Duisburg-Essen

E-Mail: lars.breuer@uni-due.de

The use of Secondary Ion Mass Spectrometry (SIMS) and Secondary Neutral Mass Spectrometry (SNMS) has become increasingly important in the characterization of materials, particularly for high-resolution imaging and depth profiling. SIMS/SNMS is a powerful tool for analyzing surfaces, interfaces, and thin films. In recent years, the development of laser post-ionization has enhanced the capabilities of these techniques, allowing for improved sensitivity and selectivity.

In this CENIDE meeting, we will discuss the determination of ionization probabilities in SIMS/SNMS and MeV-SIMS/SNMS, as well as the imaging capabilities of these techniques. We will explore the various applications of laser post-ionization, including the analysis of organic and inorganic materials. Additionally, we will discuss the future trends and potential for these techniques in the fields of materials science, biology, and environmental analysis.

Overall, this talk aims to provide a comprehensive overview of the current state of SIMS/SNMS and MeV-SIMS/SNMS with laser post-ionization, highlighting the latest developments and future directions in these exciting areas of research.



6: Gas-phase synthesis: graphene and soot evolution, coated nanomaterials, and new templating methods

Claudia-F. López-Cámara, Hartmut Wiggers

EMPI, Institute for Energy and Materials Processes– Reactive Fluids, and CENIDE, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048, Duisburg, Germany

E-Mail: claudia-francisca.lopez@uni-due.de

An overview on some of the gas-phase synthesis processes that are employed in our laboratories to produce carbonaceous materials (i.e., few layer graphene – FLG – and soot), as well as more complex structures (e.g., coated nanoparticles) is presented here. The aim is to provide a general knowledge of these processes, which use plasma, flame, and hot-wall reactors, or a combination of the three.

The first discussed study shows the synthesis of carbonaceous species within a plasma reactor [1]. The produced materials were thermophoretically sampled at different distances from the decomposition region (i.e., different heights above plasma nozzle), and their morphology evolution was studied to determine what drives the formation of graphene, soot, or both materials. Moreover, a hypothesis for the FLG formation and morphology evolution is shown [2].

Secondly, we discuss the inline formation of core-shell particles to form, e.g., $TiO_2 | SiO_2$ coreshell nanoparticles by introducing a gaseous silica precursor in the TiO_2 laden off-gas of a flame reactor [3]. The results showed that process conditions, such as coating precursor concentration and coating gas inlet velocity, determine whether (i) heterogeneous nucleation on TiO_2 particles' surface leading to homogeneously grown thin films of the coating material will occur, or (ii) homogeneous nucleation of coating material nanoparticles will occur. Using this understanding, we coated carbonaceous species (FLG and soot) with silicon [4]. The most surprising results from this latter work is that gaseous carbonaceous species react with the silicon precursor SiH_4 forming substoichiometric silicon carbides during layer formation, from which porous structures can be created using the carbonaceous materials as templates.

- [1] C.-F. López-Cámara, P. Fortugno, M. Asif, S. Musikhin, C. Prindler, H. Wiggers, T. Endres, N. Eaves, K.J. Daun, C. Schulz, *Combust. Flame* (2023, accepted for publication).
- [2] C.-F. López-Cámara, P. Fortugno, H. Wiggers, C. Schulz, *Appl. Phys. Lett.* (2023, in preparation).
- [3] C.-F. López-Cámara, M. Dasgupta, P. Fortugno, H. Wiggers, *Proc. Combust. Inst.* (2022)
- [4] P. Fortugno, C.-F. López-Cámara, J.-P. Kruse, H. Wiggers, *Microporous Mesoporous Mater.* (2023, submitted).



Postdoc Session II

7: Optical Properties of Two-Dimensional Antiferromagnetic NiPS₃ Monolayers Encapsulated by Hexagonal Boron Nitride

Pradeep Kodimana Ramakrishnan¹, Adam K. Budniak², Rajesh Kumar Yadav³, Doron Naveh³, Efrat Lifshitz² and Gerd Bacher¹

 ¹ Werkstoffe der Elektrotechnik, University of Duisburg-Essen, Duisburg 47057, Germany
² Schulich Faculty of Chemistry, Solid State Institute, Russell Berrie Nanotechnology Institute, Technion–Institute of Technology, Haifa 3200003, Israel
³ Faculty of Engineering Bar-Ilan University Ramat-Gan 5290002, Israel

E-Mail: pradeep.kodimana-ramakrishnan@uni-due.de

The interest in magnetic two-dimensional (2D) van der Waals (vdW) materials has grown immensely in recent years due to their potential applications in spin-electronic and spin-optical devices. In particular, the group of transition metal thiophosphates (MPS₃) offers ways for various spin-based applications depending on the built-in transition metal due to their chemical stability and their large spectrum of possible magnetic, electronic, and optical properties. Among the MPS₃ family, NiPS₃ is a particularly intriguing material due to an ultra-narrow and sharp photoluminescence (PL) peak that is observed at 1.4756 eV with a full width at half maximum (FWHM) of ~330 μ eV. [1,2] However, PL from atomically thin monolayer NiPS₃ have not been reported so far.

For this work, NiPS₃ crystals were synthesized via vapor transport synthesis and atomically thin NiPS₃ flakes are mechanically exfoliated onto a SiO₂/Si substrate. As monolayers of 2D materials are by nature sensitive to environmental influences, such as temperature, humidity, adsorbates, the samples are encapsulated by hexagonal boron nitride (hBN). The hBN-encapsulation provides excellent protection from environmental factors, resulting in highly stability to the monolayers of NiPS₃ even at elevated temperatures.

We present temperature dependent PL measurements of mechanically exfoliated NiPS₃ flakes with thicknesses between bulk and a monolayer, encapsulated by hBN flakes. Lithographically defined markers allow for a reproducible optical access to individual NiPS₃ flakes under various experimental conditions. The PL peak exhibits excellent monochromaticity with a near-intrinsic linewidth (~1.4 meV at temperature T of ~4 K) in the near-infrared range (with photon energy of ~1.476 eV) for the monolayer. Low temperature PL studies reveal an emission band arising from the intrinsic transition. The intensity of the narrow peak clearly decreases with the increase of temperature and vanishes at T> Néel temperature (TN, ~152 K). Temperature-dependent PL spectroscopy has been used to identify the impact of exciton–phonon interaction on the homogeneous line width broadening of the ultra-narrow PL emission. It remains ambiguous, but fundamentally important to understand, why an intrinsic transition can generate such a narrow emission at hundreds of microelectronvolts. [3]

- [1] Hwangbo, K., Zhang, Q., Jiang, Q. et al. *Nat. Nanotechnol.* **16**, 655–660 (2021).
- [2] Kang, S., Kim, K., Kim, B.H. et al. *Nature* **583**, 785–789 (2020).
- [3] Wang, X., Cao, J., Lu, Z. et al. *Nat. Mater.* **20**, 964–970 (2021).



8: Large eddy simulations of nanoparticle synthesis in spray flames

Seung-Jin Baik¹, Monika Nanjaiah¹, Patrick Wollny¹, Wlokas Irenäus¹, Andreas Kempf¹

¹ Chair of Fluid Dynamics, Institute for Energy and Materials Processes (EMPI), University of Duisburg-Essen

E-Mail: seung.baik@uni-due.de

The present work describes the development of the SpraySyn burner [1], which is utilized to investigate nanoparticle synthesis from spray flames using various diagnostic techniques and simulations. The research is part of the DFG priority program SPP 1980. Specifically, the study focuses on the formation of iron oxide nanoparticles from iron nitrate dissolved in a mixture of ethanol and ethyl hexanoic acid.

In the SpraySyn burner, the nanoparticle precursor solution is atomized via an air-blast nozzle and injected into a highly reactive environment, where it evaporates at high heating rates. The solvent itself is combustible, surrounded by a pilot flame ash shown in Figure 1 (a). The synthesis flame is investigated using large eddy simulations (LES) with the in-house code PsiPhi [2]. Lagrangian particles describe the liquid droplets, while gas-phase combustion is modeled by the flamelet generated manifold approach combined with the artificial flame thickening technique. Iron oxide nanoparticle dynamics are modeled in terms of number-, surface-, and volume-concentration by a mono-modal model [3] as shown in Figure 1 (b, c, d).

The simulated nanoparticle size will be compared to in-situ measurements performed by Suleiman [4].



Figure 1. (a) A schematic drawing of the SpraySyn burner. Instantaneous contour plots of (b) the particle number concentration NN, (c) surface area concentration NA, and (d) volume concentration NV in a burner cross section.





- [1] F. Schneider, S. Suleiman, J. Menser, E. Borukhovich, I. Wlokas, A. Kempf, H. Wiggers, and C. Schulz, Spraysyn, Review of Scientific Instruments 90 (2019).
- [2] A. Rittler, L. Deng, I. Wlokas, and A. M. Kempf, Proc. Combust. Inst. 36 (2016).
- [3] F. E. Kruis, K. A. Kusters, S. E. Pratsinis, and B. Scarlett, Aeros. Sci. Technol. 19 (1993).
- [4] S. Suleiman, M. Nanjaiah, I. Skenderovic, T. Rosenberger, F. Kunze, I. Wlokas, F. E. Kruis, H. Wiggers, and C. Schulz, Journal of Aerosol Science 158 (2021)





9: Hydrogen production via dark fermentation by bacteria colonies on porous PDMS-scaffolds

M. Vadalà¹, E. Kröll¹, M. Küppers², D. C. Lupascu¹ and R. Brunstermann²

¹ Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany

² Urban Water and Waste Management Department, Faculty of Engineering, University of Duisburg-Essen, Essen, Germany

E-Mail: miriana.vadala@uni-due.de

The development of biofuels and the question of finding renewable energy sources are important issues nowadays, due to the increasing shortage of other supplies. Hydrogen has gained very much attention as biofuel, as it is highly energetic and a clean energy source. A very interesting method to produce hydrogen is dark fermentation. It generates a clean energy from organic wastes with low value and at low energy requirements. The production of hydrogen and biohydrogen from waste and wastewaters can have a positive environmental impact in terms of creation of highly effective energy fuel and reduction of waste. Due to their nutrients, organic waste and wastewaters are suitable substrates to obtain bio-hydrogen. In this contribution we investigate the behaviour and the stability of porous scaffolds containing iron oxide particles in a dark fermentation environment and explore the possibility of hosting mixed cultures of clostridia on them, aiming to an increase in hydrogen production. The scaffolds analysed consist of polydimethylsiloxane (PDMS) containing Fe₂O₃ particles and were produced via the sugar template method. If metal oxide particles, as hematite are embedded in the scaffolds, we shall observe an increase in bio-hydrogen-production, as they can increase bacterial growth and encourage the bioactivity of species that produce hydrogen. X-ray diffraction patterns, SEM images as well as dark fermentation tests in batch procedure are presented and discussed. Bacteria colonies could be detected after long treatment in municipal wastewater and production of biohydrogen was ascertained for all samples investigated.



10: Porous polymeric multi-composites with a tailored nickel microenvironment as catalytic flow-through membrane reactors for efficient *p*-nitrophenol degradation

Lukas Fischer^{1,2,3}, Anna Volz^{1,2,3}, Ulrich Hagemann^{2,3,4}, Mathias Ulbricht^{1,2,3}

¹ Lehrstuhl für Technische Chemie II
² Center for Nanointegration Duisburg-Essen (CENIDE)
³ NETZ–NanoEnergieTechnikZentrum
⁴ Interdisciplinary Center for Analytics on the Nanoscale (ICAN)

E-Mail: Lukas.Fischer@uni-due.de

The catalytic degradation of environmental pollutants like *p*-nitrophenol is a promising approach for wastewater treatment. For this, it would be very beneficial to increase the catalytic efficiency of abundant non-noble metals and to fabricate materials that enable a continuous water treatment.



In this work, a polymer-based membrane platform was established in a novel approach to immobilize nickel nanoparticles next to an adjustable multi-composite environment that improves the nickel activity for the catalytic hydrogenation of *p*-nitrophenol using borohydride. An optimized film casting and phase separation method with polyethersulfone as matrix polymer enabled the one-step fabrication of membranes with high loadings (53 wt. %) of nickel nanoparticles, carbon nanoparticles and cationic ionomer, as well as high porosity (75 %). The addition of carbon and ionomer optimized the nickel microenvironment in the porous membranes and doubled the *p*-nitrophenol turnover frequency in batch reaction. This is likely due to the utilization of *in situ* formed hydrogen by the carbon nanoparticles and the function of the cationic ionomer to bind *p*-nitrophenol and borohydride next to active sites. Combining these synergies between the functional additives with flow through the porous catalytic membrane reactors led to up to 10 times higher turnover frequencies and to an increase of reaction rate constants normalized to the nickel mass from 0.5 s⁻¹ g⁻¹ for dispersed nanoparticles to 140 s⁻¹ g⁻¹ for the best membrane. The multi-composite membranes also exhibit exceptional stability which enabled a continuous water treatment in flow-through for high *p*-nitrophenol concentration (50 mM or 7 g/L).

As next step, the continuous *p*-nitrophenol degradation using environmentally realistic wastewater conditions will be assessed, and advanced membranes with properties tailored to this process will be fabricated. We will further use these novel multi-composite membranes to investigate the possibility to develop a combined pollutant degradation and membrane filtration wastewater treatment process.



11: Investigating the inception of carbonaceous particles: from flames to shock-tube

Can Shao, Mustapha Fikri, Christof Schulz

Institute for Energy and Materials Processes – Reactive Fluids, University of Duisburg Essen

E-Mail: can.shao@uni-due.de

Although carbonaceous particle formation in the combustion process has been studied for decades, mysteries remain especially in the transition from gas-phase molecules to carbon clusters and initial particles. There are three hypotheses for the key inception mechanism: 1) Combination of two-dimensional polycyclic aromatic hydrocarbons (PAHs) with fullerene-like structure; 2) Physical coalescence of PAHs into stacked clusters, called physical dimerization or physical inception, and 3) Chemical coalescence of PAHs into cross-linked, three-dimensional structures, named chemical dimerization or chemical inception. Unfortunately, there are no solid arguments to support each hypothesis, especially when accounting for the prevailing temperature. This talk gives an overview of experimental methods to investigate the inception of carbonaceous particles in various reaction systems.

The first part is focusing on sampling infant soot particles from well-defined flames followed by analysis using state-of-the-art mass spectrometry. We found that PAH molecules present in soot particles are all stabilizers. Kinetic Monte Carlo simulations and thermodynamic stability calculations further identify the detected PAHs as peri-condensed and without aliphatic chains. Van der Waals forces can easily link PAHs of such size and shape to form PAH dimers and larger clusters under the specified flame conditions. Our results provide direct experimental evidence that soot inception is initiated by a physical process under typical flame conditions.

The second part is about the *in-situ* laser diagnostics in a shock tube. So far, no *in-situ* experiments have been performed in high-temperature pyrolysis of hydrocarbons in the context of particle inception. This is because most pyrolysis tests were performed in heated flow reactors which are only available for *ex-situ* studies, or *in-situ* measurements in a very narrow nucleation zone in flames. Unlike flames, with narrow inception zone and temperature gradients, shock tubes provide a unique possibility to investigate particle inception through *in-situ* laser diagnostics under uniform and well-defined conditions (1400–3000 K), and in the absence of transport processes for the pyrosis of precursors.



12: Characterization of particle dynamics and orientational phenomena in soft, magnetic hybrid materials

J. Landers¹, J. Kopp¹, B. Rhein², S. Salamon¹, A. M. Schmidt², R. Müller³, H. Wende¹

¹ Faculty of Physics and CENIDE, University of Duisburg-Essen ² Department of Chemistry, University of Cologne ³ Leibniz Institute of Photonic Technology, Jena

E-Mail: joachim.landers@uni-due.de

Soft magnetic hybrids formed from magnetic nanoparticles embedded in gels, complex fluids, polymers etc. exhibit a widely tunable range of physical characteristics, combining the (visco) - elastic properties of the chosen matrix material with a response to magnetic stimuli dependent on the type of embedded particles. To harness and optimize these properties however, it is



Effects of Brownian motion and nanoparticle magnetic alignment as observed via Mössbauer spectroscopy.[1]

necessary to understand the complex particle dynamics, being affected by magnetic fields and different particle-matrix interaction as well as interparticle interaction mechanisms.

Here, we demonstrate an in-detail analysis of exemplary soft magnetic hybrids and ferrofluids using Mössbauer spectroscopy in combination with AC-susceptometry and complementary techniques. We are able to simultaneously access information on Néel relaxation, particle agglomeration and diffusion coefficients, as well as on the particles' internal magnetic structure and alignment processes.[1,2]

In an attempt to expand the functionality of magnetic hybrid materials even further, in our ongoing study we aim for the preparation and characterization of liquid-crystal (LC) based soft magnetic media, to utilize the LC mesogenes' self-ordering and response to electric fields.[3]

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Poster Session I

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1: CrTe₂ as a two-dimensional layer for topological magnetism in complex heterostructures

Nihad AbuAwwad^{1,2,*}, Manuel dos Santos Dias³, Samir Lounis^{1,2*}

 ¹ Peter Grünberg Institute (PGI), FZJ, 42425 Julich, Germany
² Faculty of Physics, University of Duisburg-Essen, 47053 Duisburg, Germany
³ Scientific Computing Department, STFC Daresbury Laboratory, Warrington WA4 4AD, United Kingdom

E-Mail: *n.abuawwad@fz-juelich.de, s.lounis@fz-juelich.de

The discovery of two-dimensional (2D) van der Waals magnetic materials and their heterostructures provided an exciting platform for emerging phenomena with intriguing implications in information technology. $CrTe_2$ is a particular example that hosts complex magnetism strongly intertwined with its crystal structures [1,2]. Here, based on a multiscale modelling approach that combines first-principles calculations and a Heisenberg model, we demonstrate that interfacing this 2D layer with various Te-based layers hosting heavy or light elements enables the control of the Dzyaloshinskii-Moriya interaction and magnetic anisotropy energy of the whole heterostructure, and thereby the emergence of new magnetic phases of matter, which are of topological nature such as skyrmions and merons.

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2: Influence of superconductivity on Heisenberg's exchange and the Dzyaloshinskii–Moriya interaction

Uriel A. Aceves Rodriguez^{1,2}, Filipe Guimarães³, Samir Lounis^{1,2}

¹ Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

² Faculty of Physics & CENIDE, University of Duisburg-Essen, 47053 Duisburg, Germany ³ Jülich Supercomputing Centre, Forschungszentrum Jüllich & JARA, 52425 Jülich, Germany

E-Mail: u.aceves@fz-juelich.de

Magnetic exchange interactions (MEI) are instrumental for the development of new quantum technologies based on magnetism, and it is essential to have tools to analyze them based on realistic descriptions of the electronic structure of materials. When in combination with superconductivity, magnetic materials have a potential impact on topological quantum computing based on Majorana Zero Modes as qubits [1].

In this work, we investigate a prototypical Nb/Mn (110) system using a multi-orbital tight-binding approach, with parameters obtained from first principle calculations. We develop a theoretical framework to calculate the MEI within the Bogoliubov-de Gennes method [2] which is used to obtain the ground state properties of the magnetic structures interfaced with a superconductor.

We perform self-consistent calculations to assess the impact of superconductivity on the MEI, exploring different strengths of the superconducting state in Nb. Small gap sizes lead only to minimal corrections on the interactions, which have no significant effect over the ground state. However, for large superconducting strengths we find that the impact on the Heisenberg's exchange is large, and the magnetic ground state changes from antiferro- to ferromagnetic. For the Dzyaloshinskii–Moriya interaction we observe a change in chirality at large superconducting gap sizes. The method developed in this work is general and may help future investigations to analyze magnetic textures, and nanostructures on superconductors, which are fundamental for the experimental realization of Majorana Zero Modes.

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3: Optimizing sustainable thermoelectric materials for 300-600 K applications

B. Aguiar Santos¹, A. Pereira Gonçalves¹, J. de Boor²

¹ Centro de Ciências e Tecnologias Nucleares (C2TN), DECN, Instituto Superior Técnico, Universidade de Lisboa, Portugal.

² German Aerospace Center (DLR), Institute of Materials Research, D–51147 Köln, Germany.

E-Mail: beatriz.santos@ctn.tecnico.ulisboa.pt

One of the world's greatest global issues is the energetic crisis. As we evolve and grow as a society, new technologies become available and more affordable, consequently the energetic demand increases.

In this sense, thermoelectric materials (TE), which can convert heat into electricity and viceversa through the thermoelectric phenomena, emerge as an elegant solution to mitigate this global issue, as they can be employed for power production from (waste) heat. Moreover, TE devices are maintenance-, noise- and vibration-free, easily scaled-up or down, and can be implemented to a wide range of working temperatures, thus allowing them to be used in various fields ranging from biosensors to space applications [1].

Nevertheless, most commercially available TE devices are composed of costly and/or toxic elements (e.g. Bi₂Te₃, PbTe) [2]. Hence, it is imperative to find more sustainable solutions, with a competitive thermoelectric performance.

Magnesium-based materials, such as Mg_2X (X=Si,Sn), seem to fit the requirements, they are made from earth-abundant, cheap and environmental friendly elements, with a good thermoelectric performance at high temperature (600-800 K) [3].

The aim of this work is to optimize Mg_2X ($Mg_2Si_{1-y}Sn_y$, y=0.3-1.0) for usage between room temperature and 600 K, i.e. shifting the optimum working range to lower temperatures and hence creating a suitable TE material to replace Bi_2Te_3 .

For this purpose, a prediction model was employed based on the Boltzmann transport equation, which allows the prediction of optimum thermoelectric properties based on the charge carriers concentration, and exploration of the formation of a solid-state compound throughout the whole composition [1]. Additionally, different synthesis and sintering routes were tested to evaluate their effect on the thermoelectric properties.

Thus, by changing the carrier concentration, the model is able to give the corresponding optimized thermoelectric properties for a certain temperature range and according to the predictions of the model, one can adjust the composition to shift the band gap (decrease it), towards Mg₂Sn, favoring improved thermoelectric properties at lower temperatures.

Results based on the prediction of the model and experimental data will be shown in the poster.

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4: Emergence of zero-field non-synthetic single and interchained antiferromagnetic skyrmions in thin films

<u>Amal Aldarawsheh^{1,2*}</u>, Imara Lima Fernandes¹, Sascha Brinker¹, Moritz Sallermann^{1,3,4}, MuayadAbusaa⁵, Stefan Blügel¹, and Samir Lounis^{1,2*}

¹ Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

² Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany ³ RWTH Aachen University, 52056 Aachen, Germany

⁴ Science Institute and Faculty of Physical Sciences, University of Iceland, VR-III, 107 Reykjavík, Iceland

⁵ Department of Physics, Arab American University, Jenin, Palestine

E-Mail: *a.aldarawsheh@fz-juelich.de; s.lounis@fz-juelich.de

In future information technologies, Antiferromagnetic (AFM) skyrmions are considered to be optimal topological magnetic bits with localized properties. In contrast to ferromagnetic (FM) skyrmions, they are immune to the skyrmion Hall effect [1, 2], might offer potential terahertz dynamics [3] while being insensitive to external magnetic fields and dipolar interactions. Although observed in synthetic AFM structures [4] and as complex meronic textures in intrinsic AFM bulk materials [5, 6], their realization in non-synthetic AFM films, of crucial importance in racetrack concepts, has been elusive. In this work [7], we unveil their presence in a row-wise AFM Cr film deposited on PdFe bilayer grown on fcc Ir(111) surface. Using first-principles, we demonstrate the emergence of single and strikingly interpenetrating catenated AFM skyrmions, hosted by PdFe. Besides the identification of an ideal platform of materials for intrinsic AFM skyrmions, we anticipate the uncovered knotted solitons to be promising building blocks in AFM spintronics.

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5: Size Matters: Investigating the Impact of Si/C Supraparticles Size on the Lifetime of Li-ion Battery Half-cells

<u>Adil Amin</u>,^{1,z} Moritz Loewenich,² Julius T Kahl,¹ Mena-Alexander Kräenbring,¹ Hartmut Wiggers,^{2,3} Fatih Özcan,¹ and Doris Segets^{1,3,z}

¹ Institute for Energy and Materials Processes – Particle Science and Technology (EMPI – PST), University of Duisburg-Essen (UDE), Germany ² Institute for Energy and Materials Processes – Reactive Fluids (EMPI – RF), University of Duisburg-Essen (UDE), Germany ³ Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen (UDE), Germany

^z Email: adil.amin@uni-due.de, doris.segets@uni-due.de

Developing high-performance dense anodes for lithium-ion batteries (LIBs) with good cycling stability is a current research hotspot. In our recent study¹, we showed that the dilemma of high surface area and low coating density (hinderance in achieving high volumetric energy density batteries) introduced when using nanosized aggregates is partially solved by hierarchical structuring via spray drying by which supraparticles (Fig.1a) composed of nanostructured aggregates are produced. We showed that the cycle life of silicon-based anode materials can be improved by structuring into supraparticles.

However, beyond phenomenological proof of principles, understanding the effect of supraparticles size distribution on electrochemical performance (EC) is of great significance for making Si-based active materials ready for the LIBs industry. In this study, correlations between supraparticles median sizes/size distributions and other supraparticles properties such as their BET surface area, slurry rheology, coated layer quality including electrochemical lifetime of half-cells were developed. Further results showed that large median sizes of supraparticles improve the life cycle of Li-ion half cells as shown in Fig.1b. However, there exists an optimum median size above which the cycling stability of the supraparticles in half-cells starts to decrease.



Figure 1. a) Exemplary SEM image of supraparticles and nanoparticles (inset) and b) Life cycle of Li-ion half cells in dependence of Si/C supraparticles median sizes

To conclude, supraparticles exhibit properties (e.g., high layer stability, low surface reactions) that clearly go beyond those of the individual nanoparticles alone. Understanding the role of supraparticles sizes in generating anodes with a hierarchical structure gives great promises. Finally, this study enables us to further unravel process-structure-property relationships and understand the physics behind the improved EC performance of supraparticles.



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6: Investigation of the chemical interaction of iron(III) nitrate in 1-butanol and laminar fuel gas-oxygen flames by laserinduced fluorescence spectrometry

<u>S. Apazeller¹</u>, S. Karaminejad¹, M. Nanjaiah², I. Wlokas^{2,3}, T. Endres¹, H. Wiggers^{1,3}, C. Schulz^{1,3}

¹ EMPI, Institute for Energy and Material Processes – Reactive Fluids
² EMPI, Institute for Energy and Material Processes – Fluid Dynamics
³ CENIDE, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Duisburg
47057 Germany

E-Mail: sascha.apazeller@uni-due.de

Spray flame synthesis offers a flexible and efficient method for the formation of functional oxide nanoparticles derived from combustible solutions of appropriate precursors [1]. To determine the synthesis parameters required for the desired product, a detailed understanding of all the involved sub-processes during the combustion of the precursor solutions is necessary. Little has been learned about the interaction between precursor and flame chemistry so far since detailed modeling of the chemical processes with this complex geometry is hardly possible to compute.

A newly developed flat flame burner can feed aerosols from ultrasonically atomized precursor solutions over a large area of a flat flame, forming an approximately smooth, one-dimensional geometry with vertical stretching of the reaction zones at low pressure (40 mbar) [2]. This enables the study of successive processes in the flame along the height axis with good spatial resolution, and the obtained measurement data can be used to develop and validate reaction mechanisms.

This contribution presents the study of CH_4/O_2 as well as H_2/O_2 flames to which an aerosol of iron(III) nitrate dissolved in 1-butanol was added. Different flame parameters were analyzed by laser-induced fluorescence spectrometry (LIF), from which the relative OH and Fe concentrations, flame temperatures with OH LIF, and chemiluminescence of CH* and OH* were determined. The results were compared with 1D and 3D simulations.

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7: Focused-Ion-Beam Induced Defect Emitters in Hexagonal Boron Nitride

F. Schaumburg, M. Zöllner, V. Dergianlis, D. Kaczmarek, M. P. Geller, A. Lorke, and G. M. Prinz

Faculty of Physics, University of Duisburg-Essen and CENIDE

E-Mail: guenther.prinz@uni-due.de

Van der Waals materials gained great interest since the first realization of graphene by Andre Geim and Konstantin Novoselov in 2004 [1]. Hexagonal boron nitride (hBN) belongs to this group of 2D materials. In the beginning, hBN was intensively used to encapsulate other 2D materials to drastically improve their electronic and optical properties. But hBN itself is gaining more and more interest, since it can host optically active single defects, that show single photon emission even at room temperature [2-6]. This property is one key aspect for the realization of quantum communication, which makes hBN a potential candidate for a building block for this technology.

In this presentation, we show how we can create optically active defects in the infrared spectral region using a focused ion beam (FIB). We find photoluminescence peaking at ~820nm. Up to now, the luminescence is rather broad, which suggests that multiple defects have been created. But we also find sharper emission lines in the visible spectral range stemming potentially on the one hand from natural defects and on the other hand from FIB preparation. g²-measurements suggest that they might show single photon emission.

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8: Understanding the mechanochemical approach and structureactivity relationships of transition metal oxides as electrocatalysts

<u>Mohit Chatwani</u>¹, Adarsh Jain¹, Vineetha Vinayakumar¹, Timo Wagner², Christian Marcks³, Nicolas Wöhrl^{2,4}, Anna K. Mechler³, Doris Segets^{*,1,4}

¹ Institute for Energy and Material Processes – Particle Science and Technology (EMPI-PST), University of Duisburg-Essen (UDE), Duisburg, Germany ² Faculty of Physics, University of Duisburg–Essen (UDE), Duisburg, Germany; ³ Electrochemical Reaction Engineering, RWTH Aachen University, Aachen, Germany;

⁴Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen (UDE), Duisburg, Germany

E-Mail: mohit.chatwani@stud.uni-due.de

Generating energy has been a necessity from the past decades. Water electrolysis is one of the sustainable ways to produce hydrogen as a fuel since there is zero carbon emission, however, it requires high energy input which restricts its use in large scale applications.^[1] Noble metals have the potential to overcome this and are thus a viable option, but they are usually expensive and scarce making them inaccessible, in particular for industrial applications. Switching to non-noble metal-based materials is a feasible alternative solution but still lacks processing highly efficient anode materials for industrial settings.

Here, the process chain of electrode fabrication was systematically analyzed using Ni- and Cobased commercial oxide powders. Preliminary dispersion characterization pointed towards the further need of ink optimization due to instability in multiple solvents. Therefore, a mechanochemical approach was used to overcome this problem. By ball milling, chemical reduction and lower particle size was achieved with a concomitant increase in dispersion stability as confirmed by analytical centrifugation. Altering of both, the size and the phase of the powders was further confirmed by transmission electron microscopy with energy dispersive X-ray spectroscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. Selected dispersions were coated on Ni plates through ultrasonic spray deposition to obtain electrodes that underwent post-heat treatments for further improving the stability of the catalyst layers. Using a newly developed approach that includes statistical analysis, image processing, and computer vision techniques, the structural features of the catalyst layers were comprehensively analyzed using atomic force microscopy. Finally, these electrodes were tested for their functionality as anode catalysts for alkaline water electrolysis, where their physicochemical properties were correlated with their electrochemical activity.

In conclusion, an improvement in the process efficiency by analyzing and optimizing commercially available electrode materials is presented here. The mechanochemical activation of the material via ball milling opens up several degrees of freedom beyond catalyst composition to end up with competitive and non-noble metal based materials.

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9: Direct numerical simulations of particle-forming flames

L. Cifuentes, I. Wlokas, A. Kempf

Chair for Fluid Dynamics, Institute for Energy and Materials Processes, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany

E-Mail: luis.cifuentes@uni-due.de

This work investigates the effect of turbulence on particle-forming flames via 2D-3D direct numerical simulations. The analysis is performed at different Reynolds numbers and using different configurations (flame-vortex interaction, turbulent planar jet flames, and pulsating flames). The contributions to the change in particle concentration due to diffusion, coagulation, and nucleation are analyzed in detail. The influence of the complex normal and tangential strain rates that control the thickness of particle-loaded zones are also evaluated. This information provides physical insights into how the turbulent flow process affects particle- forming flames and is used with the aim of developing future modeling for the simulation of nanoparticle synthesis.

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10: Niobium Doping-Induced Ambipolar Transport in MoS₂ for Optoelectronic Devices

Osamah Kharsah, Stephan Sleziona, Marika Schleberger

University of Duisburg-Essen

E-Mail: osamah.kharsah@uni-due.de

Atomically thin molybdenum disulfide is a two-dimensional material with excellent electronic properties, thermal stability, and mechanical durability, making it an important disruptive technology in the field of optoelectronics. However, its strong n-type conductivity has impeded its development and use in p-n junction structures. To overcome this limitation, substitutional doping can be used to controllably p-dope MoS_2 . In this study, direct growth of niobium-doped monolayer MoS_2 was carried out, and the doping effect was investigated using Raman and photoluminescence spectroscopy. The annealing of a niobium-doped MoS_2 field-effect transistor led to the activation of doping sites, resulting in ambipolar transport behavior instead of the previous n-type behavior. Additionally, the sulfur annealing compared to the wide hysteresis seen before. These findings indicate that substitutional doping can potentially solve the problem of strong n-type conductivity in MoS_2 and pave the way for the development of the next generation of optoelectronic devices.



11: A DNA logic gate for sensing and transmitting molecular information

Sayantan De and Barbara Saccà*

ZMB and CENIDE, Faculty of Biology, University Duisburg-Essen

E-Mail: sayantan.de@uni-due.de, barbara.sacca@uni-due.de

The aim of this project is to design DNA-based nanosensors that can sense specific molecular information and transform it into a unique output signal through a programmable reaction cascade. Being the concept of general applicability, the DNA nanosensor can be tailored to perform ad-hoc tasks. Here we constructed an AND logic gate for the specific detection and targeted killing of cancer-specific immune cells. We then implemented the logic gate within a DNA-confined space with the aim to study the transmission of molecular information along prescribed nanosized distances and in different crowding conditions, thus providing initial tools for the mimicking and understanding of naturally occurring phenomena.

As a proof-of-principle, specific antibodies are functionalized with two DNA strands, A and B as inputs for the DNA logic gate system. This latter is programmed to work as an AND logic gate, meaning that the output signal will be generated only if both A and B are present. Thus, given a target cell carrying the surface antigens, the addition of the AND logic gate will initiate a cascade of single-strand displacement reactions [1] that eventually leads to the binding of a gold nanorod. The targeted cells will be killed by photothermal treatment using gold nanorods specifically localized on the cell surfaces. We aim to apply this system to target tumour- promoting macrophages and neutrophils as a potential tool for cancer diagnosis and treatment [2].

We are currently implementing a modified version of the logic gate to perform a reaction cascade within a DNA origami cage [3]. By placing the input strands at pre-defined intermolecular distances and in presence of different levels of crowding agents, the aim is to investigate the diffusion of small molecules within a nanoconfined space with programmable inner features. Finally, the cascade will be designed to sense an incoming signal at one side of the compartment and transmit the output signal on the opposite side. This will initiate a hybridization chain reaction [4] resulting in the formation of long DNA filamentous appendages at one extremity of the DNA cage, thus mimicking - in a very simple fashion - the growth and possibly the biased diffusion of bacteria cells [5].

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12: On the stability of thermoelectric materials: investigating Mg diffusion in Mg₂(Si,Sn) at room temperature

<u>Amandine Duparchy¹</u>, Radhika Deshpande¹, Sanyukta Gosh¹, Mohamed Abdelbaky², Wolfgang Mertin², Eckhard Müller^{1,3}, Johannes de Boor^{1,4}

 ¹ German Aerospace Center, Institute of Materials Research, Cologne, D-51147, Germany
² University of Duisburg-Essen, Werkstoffe der Elektrotechnik and CENIDE, D-47057 Duisburg, Germany
³ Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, D-35392 Giessen, Germany

⁴ University of Duisburg-Essen, Institute of Technology for Nanostructures and CENIDE, D-47057 Duisburg, Germany

E-Mail: amandine.duparchy@dlr.de

Due to their ability to convert (waste) heat into electricity, thermoelectric (TE) generators are highly attractive in fields like automotive or aerospace. Magnesium silicide- stannide Mg₂(Si,Sn) solid solutions are part of a very interesting family of TE materials due to their low density, as well as cheap, abundant and nontoxic elements. Though Mg₂(Si,Sn) TE properties have been optimized [1, 2] and thermoelectric generators have been fabricated successfully [3], previous investigations have also shown limited stability against oxidation in air at high temperature (>430°C) and against Mg loss in inert atmosphere [4, 5]. By integral measurement of the thermoelectric properties we furthermore found that under certain conditions the material also undergoes changes at room temperature (RT).

We focus our stability investigations on Mg-poor p-type $Mg_2Si_{0.3}Sn_{0.7}$ and Mg-rich $Mg_{2+\delta}Si_{0.3}Sn_{0.7}$ due to their high thermoelectric performance and previous implementation in prototype devices. The samples were synthesized via a melting process and therefore show some compositional variation on a µm-scale. Samples were then stored in different conditions at RT (air, inert or water) to investigate the impact of the storage condition over time and establish a related mechanism. Integral measurement of the TE properties shows that Mg-rich sample deteriorate over time (decrease of charge carrier concentration) while Mg-poor samples remain stable. Inert stored samples are expected to remain stable compared to air stored sample, and yet, it showed slight deterioration over time.

SEM/EDX combined with AFM and Kelvin Probe Force microscopy were used to analyze the microstructural changes at the surface of the samples. For samples stored in air they reveal a surface degradation which is clearly selective to Si:Sn content and MgO formation on Sn-rich reasons of the sample surface.

Local scanning of the Seebeck coefficient across the depth of the sample shows that the change in properties is a surface effect, indicating a diffusion mechanism towards the surface as driving force for the material change.

This work not only establishes the effect of storing conditions on TE properties and microstructure but also proves that it is a magnesium related mechanism comprised of several steps: (i) magnesium evaporation/loss (Mg_{2+δ}X \rightarrow Mg₂X + δ Mg), (ii) magnesium diffusion towards the surface inside the bulk and (iii) magnesium oxidation at the surface (Mg + O₂ \rightarrow MgO). Such correlation between Mg content and TE properties will be further investigated in future work to study the possible synthesis of Mg-poor n-type solid solution to avoid Mg excess in TEG and such degradation over time.



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13: Photodegradation of plasticizer using doped Bismuth Ferrite nanoparticles

<u>Astita Dubey</u>,^{1*} Mohd. Shoaib,^{2,3} Muntjeer Ali,³ Ulrich Hagemann,⁴ Ahmad. Kazmi,³ Raj K. Dutta,² Marianela Escobar Castillo,¹ Vladimir V. Shvartsman,¹ Doru C. Lupascu¹

¹ Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141 Essen, Germany

² Department of Chemistry, Indian Institute of Technology Roorkee, 247667 Roorkee, India ³ Environmental Engineering Group, Civil Engineering Department, Indian Institute of Technology Roorkee, 247667 Roorkee, India

⁴ Interdisciplinary Center for Analytics on the Nanoscale (ICAN) and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1-21, 47057 Duisburg, Germany

E-Mail: astita.dubey@uni-due.de

Our study demonstrated that doped-Bismuth Ferrite Nanoparticles (BFO NPs) functionalized with Graphene Oxide (GO) showed remarkable efficacy in degrading plasticizer under UV light irradiation within 3 hours. Plasticizers are widely used in numerous industrial and consumer products. However, its use has been linked to potential endocrine-disrupting effects, posing a severe risk to both human health and the environment.

Photodegradation has been identified as a promising approach to mitigate the negative impact of phthalates. BFO NPs, in particular, have been found to be effective photocatalysts for phthalate degradation. In this study, the BFO NPs were doped with additional elements and functionalized with GO to enhance their photocatalytic activity.

We have analysed the degraded by-products of phthalate using Gas Chromatography-Mass Spectrometry (GCMS) technique, revealing that the photodegradation process resulted in the formation of various intermediate by-products. The study's findings suggest that doped-BFO NPs functionalized with GO could be a potential solution to mitigate the harmful impact of phthalates on human health and the environment.




14: Laser-optical *in situ* detection and imaging of gas-borne heteroaggregate formation

Felix Luc Ebertz¹, Torsten Endres¹, Christof Schulz¹

¹ Institute for Energy and Materials Processes – Reactive Fluids

E-Mail: felix.ebertz@uni-due.de

Hetero-aggregate formation refers to bringing particles of different materials together and creating unique physical and chemical properties. Hetero-aggregating appears, e.g., in particle-forming reaction processes like mixing aerosols from individual synthesis pathways. The optical *in situ* detection of such gas-borne hetero-aggregate formation provides valuable data to support the development of models and scale-up processes in realistic-sized *apparatus*. Therefore, this work aims to enable an *in situ* observation of interacting aerosols. The illustration in fig. 1 points out the concept of the investigated hetero-aggregation detection method.

Figure 1: Basic illustration of the hetero-aggregation detection method based on pump-probe laser



Soot/carbon black \rightarrow

interaction.

The detection concept to be demonstrated here relies on a pump(IR)-probe(UV) laser excitation schema for selective detection of hetero-aggregates. In the present case, premixed heteroaggregates of carbon black (CB) and ZnO:Zn are investigated. We are currently investigating this approach as the first method for *in situ* detection of gas-borne heteroaggregates. The material system (carbon black/ZnO:Zn) was selected here specifically to demonstrate the detection concept. The detection is based on this concept: Infrared laser light (1064 nm) is absorbed by CB to increase its particle temperature. Subsequentially, the thermal energy of CB is transferred to ZnO:Zn via heat conduction. CB temperatures lower than ≤3300 K favor the process of heat conduction and ensure that CB does not evaporate [1]. CB transfers thermal energy to the ZnO:Zn, which then increases in temperature. Exciting the ZnO:Zn with a probe UV laser pulse (355 nm) causes the ZnO:Zn to emit phosphorescence. Since ZnO:Zn is a thermographic phosphor, its light emission is temperature dependent and red-shifts with increasing temperature (central peak position at 380 nm for 300 K). This temperature increase of ZnO:Zn is used here as an indicator for hetero-aggregation. The influence of cross-talk between the different laser pulses has to be considered. This is done by a difference detection schema. Therefore, the UV laser runs at 10 Hz while the IR laser runs at 5 Hz, ensuring that only every second UV laser pulse detects the heated state of ZnO:Zn, and the signal before can be used as background. The poster shows results on spectroscopic detection and imaging results using this detection method.

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15: Multi-line laser-induced fluorescenc temperature imaging with LIFSim 4.0

A. El Moussawi^{1,2,3}, T. Endres^{1,2,3}, S. Karaminejad^{1,2,3}, J. Menser^{1,2,3}, T. Dreier^{1,2,3}, C. Schulz^{1,2,3}

¹ EMPI-RF, Institute for Energy and Materials Processes – Reactive Fluids
 ² CENIDE, Center for Nanointegration Duisburg-Essen
 ³ University of Duisburg-Essen, 47057 Duisburg, Germany

E-Mail: abbas.moussawi@uni-due.de

Laser-induced fluorescence (LIF) is a non-invasive optical diagnostic used in reactive media to measure physi-cal properties such as temperature and species concentrations. This provides important information for a crucial understanding of flame chemistry and for developing reaction mechanisms. Using laser-sheet illumination and intensified cameras as detectors allows temperature and species concentration imaging for flame characteriza-tion. An in-house modular software library, LIFSim 4.0, is developed using MATLAB for simulating NO, SiO, and OH excitation spectra. Spectral analysis tools were also implemented to interrogate and analyze spectral regions for temperature sensitivity. The library includes fitting functions optimized for enhancing and accelerat-ing the postprocessing of 2D-LIF spectra.





16: Non-equilibrium charge, spin and energy transfer at interfaces revealed by ultrafast spectroscopy

Andrea Eschenlohr¹

¹ Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

E-Mail: andrea.eschenlohr@uni-due.de

Heterostructures offer functionality due to well-controlled material properties. Excitation with femtosecond laser pulses further promises to extend this functionality to ultrashort timescales in e.g. future ultrafast spintronics devices [1]. In order to exploit and control the transient, non-equilibrium state after optical excitation, the key challenge is to identify and separate the different competing microscopic processes involving the charge, spin and lattice degrees of freedom on their intrinsic timescales. In heterostructures, transport processes further become important, and the interface properties are expected to modify the spectrum of excitations as well.

I will give an overview over the analysis of the microscopic processes underlying light-induced dynamics in heterostructures by means of femtosecond time-resolved pump-probe spectroscopy: Time-resolved interface-sensitive nonlinear spectroscopy allows to identify how ultrafast spin dynamics at ferromagnet/metal interfaces are determined by a competition of spin-dependent charge transfer and dissipation of spin angular momentum mediated by spin-orbit coupling already on timescales below 100 fs [2], which limits the non-equilibrium spin injection efficiency [3]. Element-sensitive, femtosecond time-resolved x-ray absorption spectroscopy (XAS) makes it possible to track energy transfer across the interfaces of metal/insulator heterostructures through characteristic spectral signatures [4, 5]. I will show how time-resolved XAS illuminates the importance of non-thermal lattice excitations [4] and even allows to identify the role of electronic correlations in non-equilibrium dynamics [6].

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17: Time-Resolved X-ray Microscopy: An element-specific pathway to decipher picosecond dynamics on the micro- and nanoscale

<u>Thomas Feggeler</u>^{1,2,3}, Johanna Lill⁴, Damian Günzing⁴, Ralf Meckenstock⁴, Detlef Spoddig⁴, Benjamin W. Zingsem^{4,5}, Maria V. Efremova^{6,7,8}, Santa Pile⁹, Taddäus Schaffers⁹, Sebastian Wintz^{10,11}, Markus Weigand¹¹, Andreas Ney⁹, Michael Farle⁴, Heiko Wende⁴, Katharina J. Ollefs⁴, Hendrik Ohldag^{3,12,13}, David Shapiro³, Roger Falcone^{1,2}

¹ Department of Physics, University of California Berkeley, Berkeley CA 94720, United States ² STROBE NSF Science and Technology Center on Real-Time Functional Imaging

³ Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley CA 94720, United States

 ⁴ Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany
 ⁵ Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

⁶ Department of Chemistry & TUM School of Medicine, Technical University of Munich, 81675 Munich, Germany

⁷ Institute for Synthetic Biomedicine, Helmholtz Zentrum München, 85764 Neuherberg, Germany

⁸ Department of Applied Physics, Eindhoven University of Technology, 5600 MB Eindhoven, Netherlands

⁹ Institute of Semiconductor and Solid-State Physics, Johannes Kepler University, 4040 Linz, Austria

¹⁰ Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Germany

¹¹ Helmholtz Center Berlin, 12489 Berlin, Germany

¹² Department of Material Sciences and Engineering, Stanford University, Stanford CA 94305, United States

¹³ Department of Physics, University of California Santa Cruz, Santa Cruz CA 95064, United States

E-Mail: tfeggeler@berkeley.edu

This presentation will introduce the time-resolved sampling technique developed for STXM and X-ray Ptychography/Tomography at the Advanced Light Source (ALS) in the scope of the STROBE NSF Science and Technology Center on Real-Time Functional Imaging, and the importance of such time-resolved measurement techniques for future X-ray sources like the upgraded ALS-U. The functionality of the technique will be exemplarily shown on micro- and nanostructured magnetic materials under dynamic excitations.

Element-specific and localized insights in (dynamic) magnetic properties are a key to the understanding of the functionality of multi-element micro- and nanostructures in e. g. magnetic medical and information technology approaches [1-3]. By employing the X-ray Magnetic Circular Dichroism (XMCD) effect [4] Scanning Transmission X-ray Microscopy (STXM) provides localized information on orientation and size of magnetic moments with spatial resolution below 20 nm within a wide range of X-ray absorption energies. Combining the STXM technique with a phased-locked-loop based detection scheme allows to phase-resolved sample magnetization dynamics up to 10th of GHz with picosecond interval between the imaged phases, which is demonstrated on Py/Co microstructures [5], Py stripe ensembles [6] and magnetite nanoparticle chains inside magnetotactic bacteria *Magnetospirillum Magnetotacticum* [7], revealing uniform and non-uniform resonant responses in agreement with micromagnetic simulations.

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18: PFD-filled polypeptide capsules as artificial oxygen carriers

Huayang Feng¹, Jürgen Linders¹, Eva Hillen², Christian Mayer¹

¹ Institute for Physical Chemistry, CeNIDE, University of Duisburg-Essen, Universitaetsstr. 5, 45141 Essen, Germany

² Institute for Physiological Chemistry, University Hospital Essen, University of Duisburg-Essen, Hufelandstr. 55, 45122 Essen, Germany

E-Mail: christian.mayer@uni-due.de

Artificial oxygen carriers (AOCs) based on perfluorocarbons (PFCs) have been studied and developed for about half a century [1,2]. Since PFCs are not dissolvable in blood, they are often emulsified or encapsulated before intravenous administration. In this work, it is attempted to prepare capsules from a synthetic protein as a membrane material. For that purpose, triblock polypeptides consisting of a hydrophilic aspartate block, a hydrophobic phenylalanine block, and a central cysteine block for cross-linking are synthesized to form spherical solid protein-like capsule walls around PFC droplets.

Polypeptides are synthesized through polymerization of activated N-phenoxycarbonyl amino acid derivatives [3]. Capsules are prepared by cross-linking of amphiphilic polypeptide molecules around PFD droplets that are obtained by ultrasonication. Most of the capsules exhibit a diameter that ranges from 100 nm to 1000 nm. The capsule wall exhibits sufficient mechanical strength for their use in dispersion but not enough to maintain the intact spherical shape after drying process. This may not really present a problem, as the planned use of the capsules for blood replacement would not include a drying step.

As observed by NMR spectroscopy, the capsule wall allows for fast gas exchange and the gas exchange is completely reversible. The capsules also exhibit a large self-diffusion constant as around $2.05*10^{-12}$ m²/s in aqueous solution, which guarantees efficient oxygen delivery in the environment of a blood vessel. The capsules also exhibit small cytotoxicity when tested on cell cultures.

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19: Volumetric imaging of the SpraySyn flame via tomographic reconstructions of emission and refractive index using multisimultaneous measurements for investigation of nanoparticle synthesis from flame spray pyrolysis

Cheau Tyan Foo¹, Fabio J. W. A. Martins¹, Andreas Unterberger¹, Khadijeh Mohri^{1,2,3}

¹ Institute for Energy and Materials Processes (EMPI) – Tomography, University of Duisburg-Essen, Germany

² Institute for Energy and Materials Processes (EMPI) – Fluid Dynamics, University of Duisburg-Essen, Germany

³Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany

E-Mail: cheau.foo@stud.uni-due.de

Tomographic imaging using multi-simultaneous measurements (TIMes) [1] is performed on the SPP1980 SpraySyn burner [2] (first and second versions) under several operating conditions to analyse the flame morphology and its potential impact on the flame spray pyrolysis [3]. Three types of single-shot and time-averaged 3D fields were obtained concurrently: (a) CH* chemiluminescence (linked to the flame front), (b) atomic and/or molecular emission from vaporized salts that were seeded into the liquid solution (related to the hot spray flame products) (Fig.1), and (c) refractive index measurements (which reflect changes in temperature, pressure and species concentration) [4,5,6]. The fields reveal structural detail with regions of mixing and interaction between the flame front, spray stream and envelope of hot gases, and aids in overcoming ambiguous interpretations from line-of-sight or planar measurements. The averaged reconstructions of investigated spray flames are asymmetric near the burner and converge towards symmetric bell-shaped distributions at downstream locations. The flame height decrease as the flow rate of the dispersion gas that aerosolises the central liquid solution increases due to faster combustion of smaller atomized droplets. The data is now made available for comparison with numerical simulations of the complex nanoparticle synthesis within the SpraySyn burner for validation purposes.



Fig.1: Single-shot and time-averaged 3D fields of CH* and Na signals under standard SF1 operational condition using the TIMes method. Normalized intensities within horizontal slices are presented at selected locations above the burner.



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20: Highly conductive copper films prepared by multilayer sintering of nanoparticles synthesized via arc discharge

Qingqing Fu, Frank Einar Kruis

Institute for Nanostructures and Technology (NST) and Center for Nanointegration Duisburg- Essen (CENIDE), University of Duisburg-Essen, Bismarckstr. 81, 47057, Duisburg, Germany

E-Mail: qingqing.fu@uni-due.de

Copper nanoparticles (Cu NPs) are a promising alternative to gold and silver NPs for the application of printing electronics [1]. The arc discharge method allows synthesizing of metallic NPs, such as copper, silver, zinc, and aluminium, with high purity and high yields [2]. It has been reported that the optimized arc discharge reactor synthesized tens of grams of copper NPs per hour [3]. Nevertheless, the application of Cu NPs in printed electronics is still limited. The main problems controlling the resistivity of printed copper patterns are the copper oxides and the pores present in the sintered film. In this work, we used copper NPs produced from an arc discharge reactor to obtain highly conductive copper films by addressing the abovementioned problems.

Our previous work showed that, by applying formic acid as a reducing gas during thermal sintering, copper oxides could be eliminated, and Cu NPs were well sintered into a connected metallic structure. In this work, by applying the multilayer sintering method, where the coating and sintering process was repeated up to four times, the porosity of copper films could be effectively reduced from 33.6 % after one-layer sintering to 3.7 % after four-layer sintering. Copper films with an electrical resistivity of 3.49 ±0.35 μ Ω·cm (two times of the bulk copper) have been achieved after four-layer sintering, while one-layer sintered copper films were measured to possess resistivity of 11.17±2.17 μ Ω·cm, as displayed in figure 1.



Figure 1. Relationship between porosity, electrical resistivity, and the number of coating and the sintered layers of copper films.



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21: Productivity increase of copper nanoparticles via laser ablation and their effect on the microstructure of permanent magnets

Philipp Gabriel¹, Franziska Staab², Anna Ziefuß¹, Karsten Durst², Oliver Gutfleisch³, Stephan Barcikowski¹

¹Technical Chemistry I, Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141, Essen, Germany

² Physical Metallurgy, Institute of Material Science, Technical University of Darmstadt, 64287 Darmstadt, Germany

³ Functional Materials, Institute of Material Science, Technical University of Darmstadt, 64287 Darmstadt, Germany

E-Mail: philipp.gabriel@uni-due.de, stephan.barcikowski@uni-due.de

Permanent magnets are used in various applications such as electric power generation, electro-mobility, and robotics. However, the high cost of rare-earth (RE) elements in permanent magnets, their supply, and their availability represent critical factors, and novel technologies to avoid or minimize the use of such strategic elements in permanent magnets need to be developed. [1] Powder bed fusion using a laser beam (PBF-LB) is an established additive manufacturing method allowing the production of complex permanent magnets under low waste conditions, which will reduce the amount of rare earth elements needed. [2] However, PBF-LB of permanent magnets typically results in low coercivity, demanding for new feedstocks to overcome this issue.

Here, nano-additivation with Cu of commercially available permanent magnetic micro powders possibly improves the magnetic properties of as-build parts by improving the grain boundary and Nd-rich intergranular phase leading to a better decoupling of the hard magnetic Nd₂Fe₁₄B phase. However, additivation using wet-chemically produced nanoparticles is known to critically reduce the flowability of the feedstocks, disabling the production of as-built parts. [3] Surfactant-free particles can be produced via laser-ablation in liquids [4], however, the laser-based production of Cu NPs typically goes along with low productivity, making the process uneconomical. [5] To overcome this issue, we performed a systematic parameter study, aiming for economically relevant outputs. Additionally, we performed loading series (0.1, 0.5, 1.0, 2.5 wt.%) of Cu on commercially available permanent magnet feedstocks to observe the effect on as-build parts, produced under full melting conditions.

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22: A Switchable DNA Origami/Plasmonic Hybrid Device with a Precisely Tuneable DNA-free Interparticle Gap

Michael Erkelenz¹, Richard Kosinski², <u>Helene Giesler</u>¹, Oliver Sritharan¹, Jesil Jose¹, Barbara Saccà², Sebastian Schlücker¹

 ¹ Department of Chemistry and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany
 ² Department of Biology and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany

E-Mail: sebastian.schluecker@uni-due.de, Barbara.sacca@uni-due.de

Hybrid devices comprising DNA Origami and plasmonic nanostructures in various morphologies strongly benefit from the capability of DNA nanotechnology to provide precise positioning of molecular objects. [1] Hybrid materials, especially designed for nanoparticle dimerisation, are used for sensing[2], spectroscopy [3] and biomedical applications[4]. The gap size in dimers plays a crucial role for the local electric field enhancement in the narrow gap (hot spot) upon resonant excitation[5].

Here, the design and assembly of a reconfigurable plasmonic DNA nanodevice for gold nanosphere (AuNP) dimerisation has been developed. A DNA Origami structure comprising a dynamic platform and boxes for AuNP incorporation was created (Fig. 1a). Incorporation of bare gold nanoparticles inside lidless 3D Origami boxes was performed using a thiol-based technique. To obtain dynamic properties, toehold-mediated strand displacement is employed for highly precise adjustment (sub-nanometer range) of gap distances between the two halves of the DNA platform. Based on transformation from a flexible state to five distinct states, defined gap distances between 0 and 15 nm are achieved, as evidenced by single-particle TEM and agarose gel electrophoresis (Fig. 1b). This approach enables AuNP dimerisation with a free hot spot, allowing site-specific functionalization for highly sensitive detection of molecules. Consequently, this reconfigurable hybrid device facilitates its use for spectroscopic applications such as surface-enhanced Raman scattering (SERS) and surface-enhanced fluorescence (SEF) by the controlled and reversible adjustment of interparticle distances in the range of ca. 0-5 nm and 5-15 nm, respectively.[6]



Figure 1: (a) Hybridization of DNA boxes with incorporated AuNP onto DNA platform resulting in desired hybrid device. (b) Switchable DNA platforms with varying calculated gap distances (top) and negative-stained TEM images showing the measured distances (bottom).



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23: DNA strand displacement reactions in confined nanospaces

Ivan Grishchuk, Barbara Saccà*

ZMB and CENIDE, Faculty of Biology, Universität Duisburg-Essen

E-Mail: ivan.grishchuk@uni-due.de, barbara.sacca@uni-due.de

Confinement and crowded environment are normal conditions under which chemical reactions occur in the cell. The typical sizes of membrane organelles range from about 30-50 nm for intracellular vesicles and luminal spacing of mammalian endoplasmic reticulum to about 1000 nm for exosomes [1,2].

DNA strand displacement (DSD) is the process through which two strands of DNA hybridize with each other, displacing one or more pre-hybridized strands [3]. The process can be initiated on a free single-stranded domain (toehold) and proceeds under thermodynamic control. DNA sequences can be designed to control the kinetics of the DSD reaction, thus providing a tool for the programmable control of reaction cascades in space and time.

In our study, we investigate the effect of nanoconfinement on DSD-driven reaction cascades. For this purpose, we developed a DNA duplex consisting of a long single-stranded template DNA hybridized to two strands, one of which carrying Cy5 and the other Cy3. When the strands are attached to the template, Cy5 and Cy3 are close enough to induce a Förster resonance energy transfer (FRET) effect. The addition of a trigger strand leads to DSD which results in the displacement of one of the dyed strands. The kinetics of this process was tuned by choosing appropriate design and experimental conditions and finally monitored by fluorescence spectroscopy. In the next step, we will integrate the DSD reaction within a DNA-origami cage (inner diameter is about 34 nm) and investigate the effect of nanosized compartmentalization on the kinetics of the process, thus mimicking, in a simplified version, the crowded conditions occurring within cell compartments [4]. In a long-term vision, we aim at implementing a cascade of DSD reactions, where the output of a reaction occurring in one cage serves as the input of a downstream reaction occurring in a second cage directly linked to the previous one. In this way, signals can be encoded, transmitted, and propagated over longer distances, and possibly with control over the direction of the information flow [5].

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24: ANTEMA – A tool for large-scale high-resolution transmission electron microscopy image analysis of metallic nanoparticles

Nina Gumbiowski¹, Kateryna Loza¹, Marc Heggen², Matthias Epple¹

 ¹ Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstr. 5-7, 45117 Essen, Germany
 ² Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

E-Mail: nina.gumbiowski@uni-due.de

In nanoparticle research, extensive knowledge about shape, size and structure of nanoparticles is important as these parameters determine the chemical, physical and biological properties of the particles. An important tool to gain insights into these parameters is high-resolution transmission electron microscopy (HRTEM). With high frame rates and increasing capabilities of transmission electron microscopes, a wide range of data can be generated. This is especially the case for *in-situ* experiments. However, the analysis of these images is usually done manually. This is not only a time-consuming and tedious task but also not feasible in cases where hundreds or even thousands of images have to be analyzed. Therefore, an automated image analysis process to access all the nanoparticle data generated by HRTEM is most welcome.

To facilitate such an automated HRTEM image analysis we have developed an automated nanoparticle transmission electron micrograph analysis (ANTEMA) tool. A neural network which was trained on manually labelled HRTEM images is used to perform the crucial step of separating the particles from the noisy amorphous background. The segmentation maps generated by the network are further processed by the program to remove small artifacts and boundary crossing particles as well as to separate overlapping particles. Finally, the program extracts geometric data about all particles like circularity, equivalent diameter, Feret diameter and perimeter and exports them to a datafile. This fully automated routine can analyze an HRTEM image within a few seconds which enables a large-scale evaluation of HRTEM nanoparticle image datasets and thereby gives more (objective!) insight into nanoparticle structures compared to a manual analysis.



25: Co-Creation Lab Product Innovations – From Lab discovery to business

Adrian Haag¹, Marvin Kollwitz¹, Darius Zalzadeh¹, Prof. Dr. Michael Giese^{1,2}

¹Co-Creation Lab Product Innovations, Schützenbahn 70, 45127 Essen

²Organic Chemistry, Faculty of Chemistry, University of Duisburg-Essen, Universitätsstr. 7, 45141 Essen

E-Mail: michael.giese@uni-due.de

The Co-Creation Lab Product Innovations (CCLP) is part of the technology and knowledge transfer strategy of the University of Duisburg-Essen. It is embedded in the "Zentrum für Gründungen und Innopreneurship der Universität Duisburg-Essen" (GUIDE), which is funded by the Ministry of Economic Affairs, Innovation, Digitalization and Energy of the state North Rhine-Westphalia. The goal of GUIDE is to support scientists interested in founding their own business and to help tackling the non-scientific challenges such as financing, patent law or to create a business plan for their start-up.

The CCLP is located in Essen and focuses on product innovation and material development. It assists scientist, students and employees of the university in overcoming the scientific and technical challenges that arise with inventive ideas. Our interdisciplinary team of product designers, chemists, engineers and 3D printing experts support the advancement of innovative product ideas, material development and creation of first prototypes. Various polymer 3D printing technologies such as filament extrusion, resin curing and powder printers as well as bioprinting capabilities are available.



26: FIB/TEM of a free-standing GaN Nanowire grown by Polarityand Site-Controlled Growth

Patrick Häuser¹, Werner Prost¹, Mathias Bartsch², Markus Heidelmann³, Axel Lorke², Nils Weimann¹

¹ Department of High-Frequency Electronics (BHE) ² Faculty of Physics and CENIDE ³ Interdisciplinary Center for Analytics on the Nanoscale

E-Mail: patrick.haeuser@uni-due.de

The III/Nitride semiconductors are of high interest for high power and optoelectronic devices. HEMTs and LEDs are the most commonly known applications, but the range of GaN applications is still increasing. [1] A drawback for this compound semiconductor is the lack of native substrates and large lattice mismatches of the ternary compounds, which lead to defective layers from epitaxy. Furthermore, the internal polarization and piezoelectric fields of the material have an influence on the performance of quantum devices like LEDs. The crystal defects and internal fields are limiting the performance and efficiency of devices.

A promising way to circumvent the highly mismatched epitaxy and the internal fields is the bottom up growth of nanowires. Due to the reduced lateral size of the crystal its lattice can easily relax during growth, which leads to filtering of defects. [2] Additionally, the nanowire geometry gives access to semi- and non-polar facets. A co-axial LED layer stack, for example, grown on the m-plane is not influenced by the Quantum Confined Stark Effect.

In our work we fabricate GaN nanowire LEDs by MOVPE on n-doped silicon (111) substrates. A pre-structuring by nanoimprint lithography allows for a polarity- and site-controlled growth of the nanowires. In our recent work we have prepared a TEM lamella of a free-standing nanowire LED by FIB. [3] The analysis by TEM of the substrate-nanowire interface gave a detailed insight on the growth mechanisms. The MQW structure on these structures can only be seen on the m-facet and not on the semi-polar tip of the nanowire. These results are necessary to understand and control the growth in detail.

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27: Utilization of a perfluoro decalin nanoemulsion in an *in vitro* ischemia-reperfusion-injury model in HL-1 cardiomyocytes

Jacqueline Hausherr¹, Ozan Karaman^{1,2}, Miriam Cantore¹, Katja BettinaFerenz^{1,3}

¹ Institute of Physiology, University of Duisburg-Essen, University Hospital Essen, Germany ² Institute of Physiological Chemistry, University of Duisburg-Essen, University Hospital Essen Germany ³ CENIDE (Center for Nancintegration Duisburg Essen) University of Duisburg Essen, Cerl

³CENIDE (Center for Nanointegration Duisburg-Essen) University of Duisburg-Essen, Carl-Benz-Strasse 199, 47057 Duisburg, Germany

E-Mail: jacqueline.hausherr@rub.de

The organ preservation process presents a wearisome challenge to successful organ transplantations since survival post-transplantation is directly related to donor organ quality. Profound tissue damage and organ dysfunction are associated with ischemia-reperfusion injury (IRI), which is a pathological condition inherent to the cessation of the blood flow and revascularization during an organ transplantation. Damage elicited by ischemia reperfusion (I/R) is traditionally suppressed by hypothermia. Static cold storage of organs will become obsolete as normothermic machine perfusions emerge which target oxygen shortage post-procurement and thus prevent exacerbation after reperfusion.[1] This preservation technique relies on organ perfusion solutions supplemented with red blood cell concentrates, which however are limited in availability. Albumin-derived artificial oxygen carriers (A-AOCs) based on perfluoro decalin (PFD) provide a promising alternative by circumventing the dependency on blood and associated complications. The PFD's blood-incompatibility necessitates its formulation as nano emulsion to exploit its extraordinary gas dissolving capability in medical applications.[2]

The employment of A-AOCs as a therapeutic for IRI should be tested in cell culture since they can potentially be utilized to attenuate IRI during organ transplantation. Until now, I/R cell culture models cannot be considered suitable for A-AOC testing since sedimentation effects of nanoparticular A-AOCs in a static model are not appraised. Thus, an in vitro cell culture model was developed in this project, which not only mimics the effects of ischemia-reperfusion on cells, but also facilitates the study of A-AOCs. Based on reports in literature, a simulated ischemia-reperfusion scenario was successfully established. Its ability to inflict I/R-associated injury was substantiated by measurements of cytotoxicity, apoptosis, and oxidative stress. The I/R cell culture model was then further modified to allow for A-AOC testing by introduction of spatial separation. A two-compartment cell culture was investigated appertaining to their efficacy in A-AOC-testing in I/R. The approach was proven to successfully separate A-AOCs without eliciting procedure-inherent stress factors. Further optimization was carried out based on investigations regarding the oxygen supply. In a nutshell, the *in vitro* cell culture model was successfully established. Its future application as first assessment tool to test A-AOC enriched perfusion solutions prior to ex vivo and in vivo approaches may contribute to enhancing organ preservation by driving the development of perfusion solutions.

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28: Using Gold Nanorods for Photothermal Therapy Mediated by a DNA Logic Gate on Immune Cells

Michelle Hechler¹, Sayantan De², Barbara Sacca², Sven Brandau³, Sebastian Schlücker¹

¹ Physical Chemistry, University Duisburg-Essen
 ² Bionanotechnology, University Duisburg-Essen
 ³ Otorhinolaryngology, University Hospital Essen

E-Mail: michelle.hechler@uni-due.de, sebastian.schluecker@uni-due.de

According to the International Agency for Research on Cancer, cancer fatalities will increase up to an estimated 11.4 million deaths in 2025 [1]. High relapse and death rates among certain cancer types resulted in utmost attention for this degenerative and life-threatening disease. The utilization of nanomaterials for photothermal therapy (PTT) harbors the potential to become a non-invasive treatment with high precision and control, compared to conventional cancer therapies [2].

In PTT, electromagnetic radiation is used to trigger a photosensitizer to convert energy into heat, leading to cell death in a localized area. Gold nanorods (AuNR) are an especially promising candidate for this application due to their high absorption cross section, which ensures the efficient generation of heat upon laser irradiation. Moreover, their optical resonance can be tuned to the near-infrared spectral region, necessary for sufficient tissue penetration depth, by controlling their aspect ratio during synthesis. Furthermore, AuNR are chemically inert constructs that display little immunogenicity, making them especially suitable for medical usage [3].



Tumor-specific cell receptors Fig. 2: Schematic overview of the DNA logic gate operation on two cell receptors.

In a sophisticated approach to target cancer-promoting immune cells with AuNR, a DNA logic gate is employed. Initially, antibody-DNA conjugates bind to immune cell surface receptors (see Fig. 1). These conjugates then serve as activating signals for a DNA logic gate. This logic gate is constructed to require two separate activation signals, which enable AuNR binding and subsequent cell killing upon laser irradiation. Using a set of two receptors instead of one should reduce unspecific binding and provide a more sophisticated targeting approach. Since the DNA logic gate operation proved to be challenging in cell culture studies, a synthetic cell model is employed.

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29: Lecithin-modified nanoscaled oxygen carriers

<u>Fabian Nocke¹</u>, Miriam Cantore², Marina Penzel¹, Andrea U. Steinbicker⁴, Katja B. Ferenz^{2,3}

¹ Institute of Physiological Chemistry, University of Duisburg-Essen, University Hospital Essen, Germany ² Institute of Physiology, University of Duisburg-Essen, University Hospital Essen,

Germany

³CENIDE, University of Duisburg-Essen, Germany

⁴ Goethe-University Frankfurt, Medical Faculty, Department of Anesthesiology, Intensive Care and Pain Medicine, Frankfurt, Germany

E-Mail: fabian.nocke@uk-essen.de

Perfluorocarbons (PFCs) are fully halogenated, mainly fluorinated alkanes. The strong polarized carbon-fluoro-bond and the alkane-like structure are causative for their characteristics like low surface tension, low viscosity and a high gas solubility. Additionally, PFCs are chemical and biologically inert – adjectives that makes them great artificial oxygen carrier candidates. Beside the advantages, PFCs are hydro- and lipophobic characteristics that impair solubility in blood or any other crystalloid infusion medium used in clinics as volume substitution. To enable the use of PFCs as oxygen carriers, PFCs need to be emulsified and stabilized with surfactants.^[1]

In this work, a new and optimized version of an artificial oxygen carrier based on perfluorodecalin (PFD) and the protein albumin as emulsifier was invented^[2]. The improvement concerns the shell of the particles now consisting of albumin and lecithin.

The lecithin-modified nanoscaled oxygen carrier (LENOX) was synthesized with a microfluidizer using a multicycle protocol under cooling with ice. Dynamic light scattering, oxygen release measurements with PreSens technique and a blood gas analyzer, as well as a rheometer were used as analytical methods to characterize the emulsion.

LENOX allow the use of crystalloid and colloidal solutions as dispersion media without limitations, which was impossible with prior comparable artificial oxygen carriers named "organ life fluid" (OLF).^[3] The improvement of LENOX is reflected by the newton-like viscosity and the smaller particle diameter as compared to the previous formulation OLF. Over a storage period of 42 days (static, 4°C), LENOX revealed only a slight particle growth and did not show any loss of oxygen capacity. In contrast, OLF displayed higher viscosity and a stronger particle growth than LENOX.

Overall, LENOX show improved stability in clinically relevant infusion media.

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30: Effect of artificial oxygen carriers on erythrocytes

Jan-Eric Sydow¹, Katja B. Ferenz^{1,2}

¹ Institute of Physiology, University of Duisburg-Essen, University Hospital Essen, Essen, Germany.

²CENIDE, University of Duisburg-Essen, Duisburg, Germany.

E:Mail: jan-eric.sydow@uk-essen.de

The increasing demand for erythrocyte concentrates requires further development of alternatives for blood supplies. Artificial oxygen carriers (AOCs) in the form of perfluorodecalin (PFD)-based nanocapsules with an albumin shell (A-AOCs) could represent such an alternative, as they revealed relevant oxygen transport capacity.^[1-2] When intravenously injected into patients A-AOCs come into contact with the patient's remaining erythrocytes.

In this study, the effects of artificial oxygen carriers on physiological parameters of erythrocytes were investigated. For this purpose, A-AOCs were synthesized by high-pressure homogenization of bovine serum albumin (BSA) along with PFD and mixed with human whole blood (local ethics approval no. 21-10314-BO) at a clinically relevant ratio for up to 24 h at body temperature (37 °C) and static conditions. Blood viscosity, free plasma-hemoglobin concentration, hematocrit, osmolality, glucose and lactate levels were determined to evaluate if erythrocytes remain intact and functional after contact with A-AOCs. Spectroscopic

photometry was used to detect the free plasma hemoglobin concentration. Hematocrit and osmolality were determined along with glucose and lactate levels by using a blood gas analyzer. In addition, viscosity was measured by a rheometer.

When using a 1:1 mixing ratio of human whole blood to A-AOCs, results showed an increased viscosity, which (as revealed by photometric hemoalobin determination) was due to hemolvsis erythrocytes. of the This phenomenon could attributed be to а combination of control solution (BSA) and A-AOCs as it was already increased in the control group (1:1 blood/BSA). In a more diluted (4:1 ratio) formulation, erythrocytes stayed intact for 24 h (Figure 1) and viscosity was not impaired. These positive results were supported by an increase of lactate with a simultaneous decrease in glucose concentration, indicating



Fig. 1: Free plasma-hemoglobin concentration for blood/A-AOC and blood/BSA samples in relation to mixing

physiological energy production (anaerobic glycolysis) of still functional erythrocytes. In conclusion, this study showed that erythrocytes remain functional and don't get negatively impaired in contact of small amounts of A-AOCs (4:1 ratio). Further experiments studying blood and blood vessel compatibility will help establish clinical application of this artificial oxygen carrier.

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Poster Session II

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56	Charlotte	van Halteren
57	Favour	Whyte
58	Arthur	Wieder
59	Moritz	Winterott
60	Libing	Zheng



31: Multi-line OH LIF gas-phase thermometry in a spray

Sadrollah Karaminejad*, Thomas Dreier, Torsten Endres, Christof Schulz

EMPI, Institute for Energy and Materials Processes –Reactive Fluids and CENIDE, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47057 Duisburg, Germany

E-Mail: sadrollah.karaminejad@uni-due.de

The present study investigates local gas-phase temperature for the SpraySyn standard burner using multi-line OH LIF. In this burner, a two-fluid nozzle disperses a precursor solution using a high-velocity flow of oxygen. The spray flame is stabilized by a surrounding axisymmetric lean premixed laminar methane/oxygen pilot flame. Multi-line OH-LIF thermometry is a technique that involves scanning across the OH absorption spectrum within a temperature-sensitive spectral region using a tunable laser. The fluorescence signal from all rotational lines are then fitted in a pixel-wise fashion to determine the species' rotational temperature. Resonant absorption by OH can lead to attenuation of the laser intensity and the resulting local signal intensity variations in the individual images must be corrected for. Laser attenuation was measured using simultaneous recordings of the fluorescence of two dye cuvettes illuminated with the laser beam before and after the flame. Spatial temperature maps were determined for the pilot flame and the ethanol spray flame. Effects of the dispersion gas flow rate and the addition of 2-EHA (2-ethylhexanoic acid) to the liquid were investigated. The addition of 2-EHA increased the temperature and influenced particle formation under synthesis conditions. The effect of attenuation measurement on the temperature determination is guantified and the maximum error that occurs without correction is reported. The temporal flame stability as an important factor in spray-flame synthesis of nanoparticles with specific characteristics is investigated. Multiline LIF can typically only determine average temperature fields since a dye laser must be scanned very slowly in the wavelength. Nevertheless, by evaluating the single shot statistics at one wavelength, the temperature stability can be inferred qualitatively. For this instantaneous OH-LIF single-shots for different operating conditions are recorded and statistically evaluated. The flame active time and the coefficient-of-variation are considered as two parameters to evaluate flame stability.



32: Synthesis, characterization and *in-situ heating* studies of faceted bimetallic nanoparticles

<u>Aikaterini Karatzia¹</u>, Kateryna Loza¹, Oleg Prymak¹, Marc Heggen² and Matthias Epple¹

¹ Inorganic Chemistry and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstr. 5-7, 45141 Essen, Germany

² Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

E-Mail: aikaterini.karatzia@uni-due.de

Noble metal nanoparticles attract more and more attention because they exhibit unique physical and chemical properties, due to their small size. They open several applications in several fields like medicine as they can be used as carriers for drug delivery [1]. Because of their special optical, electrical, and catalytic properties, they are extensively used in

electronics, as well as homogeneous and heterogeneous catalysis. Crystallographically faceted nanoparticles are of great interest in catalysis [2]. They can be prepared with a shell of another material which modifies and enhances their properties and make them more tunable for specific operations. Consequently, the nanoparticles can become even more versatile in a wider range of applications.

Here we present a wet-chemical synthesis of bimetallic silver-gold core-shell nanocubes, generated by a seed-mediated growth approach [3,4]. They were characterized by ultraviolet-visible spectroscopy (UV-Vis), dynamic light scattering (DLS), scanning (SEM) and transmission electron microscopy (TEM), energydispersive X-ray spectroscopy (EDX), atomic absorption spectroscopy (AAS), thermogravimetric analysis (TGA) and X-ray powder diffraction (XRD). Their thermal behavior, including morphological stability and internal crystallinity were studied in-situ at temperatures up to 1000°C experiments in SEM, TEM. and XRD. For comparison, microcrystalline silver powder and bulk silver were also studied.We could show that silver starts to sublime at temperatures above 600°C under vacuum conditions in SEM, TEM and XRD. This can be attributed to the high vapor pressure of silver. Ex situ XRD studies and TGA confirmed that the sublimation of silver nanocubes starts around



Figure 1. TEM image and EDX mapping of a gold-coated silver nanocube.650°C in vacuum due to its high vapor pressure, which is the highest of all noble metals [5,6].

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33: Ion induced defects in two-dimensional tungsten diselenide boron nitride heterostructure

Leon Daniel, Stephan Sleziona, Lucia Skopinski, Anke Hierzenberger, Jennifer Schmeink, and Marika Schleberger

Universität Duisburg-Essen

E-Mail: leon.daniel@uni-due.de

Monolayer transition metal dichalcogenides (TMDCs) like tungsten diselenide (WSe₂) are highly interesting materials for optoelectronic and valleytronic applications. We used Xe^{q+} ions with E_{kin} =180 keV to deliberately introduce defects into the WSe₂ lattice and compared its optoelectronic properties before and after irradiation with photoluminescence spectroscopy. Encapsulation in hexagonal boron nitride (hBN) isolates the WSe₂ from environmental influences like adsorbates and detrimental interactions with the widely used Si/SiO₂ substrates. We find differences in the photoluminescence response for encapsulated and non-encapsulated WSe₂, which can be explained by the encapsulation preventing saturation of the created vacancies by adsorbates. In particular, there are various localized excitonic states in our different sample systems, and we explain this observation with differing ion interactions with encapsulated and non-encapsulated WSe₂. Furthermore, we observe overall highly increased exciton lifetimes after the irradiation, likely caused by the longer lifetime of the localized excitons.



34: Additive Manufacturing of Bulk Metallic Glasses for Energy Conversion

J. Wegner¹, R. Martínez-Hincarpié², H.Schönrath¹, V. Colic^{2,3}, <u>S. Kleszczynski^{1,3}</u>

¹ Chair of Manufacturing Technology, University of Duisburg-Essen, 47057 Duisburg, Germany

² Electrochemistry for Energy Conversion, Max-Planck-Institute for Chemical Energy Conversion, 45470 Mülheim an der Ruhr, Germany

³ Center for Nanointegration Duisburg-Essen (CENIDE), 47057 Duisburg, Germany

E-Mail: stefan.kleszczynski@uni-due.de

Additive manufacturing techniques have recently been employed to overcome previous limitations in the manufacturing of bulk metallic glasses (BMGs). BMGs exhibit several desirable properties for various energy-related applications. Their amorphous nature provides more active sites for electrocatalytic reactions due compared to their crystalline counterparts. This can result in higher catalytic activity and improved performance. Moreover, the superior mechanical properties and chemical stability of AM-BMGs can improve the durability and lifespan of electrodes in harsh conditions. Therefore, AM-BMGs have the potential to revolutionize the design and manufacturing of energy conversion devices, such as fuel cells and batteries. The design freedom of AM potentially enables tailored structures and properties from the microscopic to the macroscopic scale. However, there are challenges that must be addressed before the full potential of AM-BMGs can be realized. Especially the relationship between AM processing parameters, the resulting microstructure, and the resulting electrocatalytic properties are not understood yet. Embrittlement and porosities challenge current process development and have to be addressed by further process and alloy optimization.



35: Reversible Photoalignment of Azobenzene in the SURMOF HKUST-1

T. Koehler¹, I. Strauss², A. Mundstock², J. Caro², F. Marlow^{1,3}

¹ Max-Planck-Institut für Kohlenforschung ² Leipzig Universität Hannover ³ Center for Nanointegration Duisburg Essen

E-Mail: koehler@kofo.mpg.de

Embedding molecular switches inside the pores of metal-organic-frameworks (MOFs) is a promising strategy to realize all optical switching, an important pathway to tackle the rising energy demand of everyday internet and communication technologies [1]. We mainly focus on azobenzene (AZB) and its derivatives as guest molecules, which can be photochemically switched between the stable trans- and the metastable cis-isomer. As hosts, we utilize thin films of MOFs, a hybrid material class made up of metal centers connected by organic linkers, to form wide, porous frameworks.

The optical film properties are analyzed primarily via UV/Vis spectroscopy, including angular dependent interferometry. We show that azobenzene inside the pores of MOF type HKUST-1 not only isomerizes well, reversibly changing the optical properties, but also shows the rare phenomenon of photoalignment.[2] Photoalignment is based on the transition dipole moment direction of the relevant π - π *-transition along the trans-AZB long axis. Irradiating azobenzene in the right environment with linearly polarized light will lead to a preferential orientation perpendicular to the polarization direction due to statistical processes, as shown in Fig. 1.

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Fig. 1. Trans- and cis-azobenzene isomerize under light illumination. Transazobenzene molecules are more likely to isomerize when oriented parallel to the light's polarization direction and will be aligned perpendicular to linearly polarized light over time [2].



36: Development of 3D-printed salicylimine-based fluorescent chemosensor for the detection of Aluminium lons in water

Marvin Kollwitz¹, Prof. Dr. Michael Giese¹

¹ Organic Chemistry, Faculty of Chemistry, University of Duisburg-Essen, Universitätsstr. 7, 45141 Essen

E-Mail: marvin.kollwitz@uni-due.de

Nowadays, the role of bio- and chemosensors for selective detection of relevant metal ions in water have recently attracted great attention. The frequent use of aluminium packaging in the food and pharmaceutical industry often brings people into contact with aluminium ions. After absorption, it will distribute to human cells and accumulate in the bones. Moreover AI^{3+} is carried by an iron binding protein and so it can enter the brain and reach the placenta. In addition, aluminium ions have been implicated as a causative factor of Alzheimer's disease and associated with damage to the central nervous system.[1–4]

Fluorescent molecules based on Schiff bases (SB) have attracted significant interest because of their simple synthesis, design and low cost production. SBs show a high potential use in medical and environmental research for their good ion binding affinity and fluorescent emission.[5] A new way to process these SBs is additive manufacturing (AM) or 3D-printing yielding complex functional topologies. Vat photopolymerization, a category of the AM process, generates 3D objects by selective curing of chemically modified liquid resin by exposure to light (405 nm) causing a light-activated curing step.[6]

We propose that the modification of resins (photopolymers) with Schiff base enables the direct production of highly selective and sensitive chemosensors for the detection of Al³⁺ in water. For that we use two different strategies to tackle this problem. First, the direct dissolution of the SBs in the photopolymer which is an uncomplicated way to modify the properties of the resin. Here we want to check whether this process works and how the detection of Aluminium ions in water behaves. Second, we want to modify the polymer surface so that Al³⁺ coordinates directly on the surface and induces fluorescent emission (Scheme 1). For this reason, the combination of simple and mobile production by additive manufacturing of chemosensors for the detection of aluminium ions in water is the next step towards a healthier lifestyle.



Scheme 1: Synthesis strategy for the surface modification of the 3D printed Chemosensor



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37: Synthetic steps to prepare chiral ultrasmall gold nanoparticles

Kathrin Kostka¹, Katrin Steiger², Gebhard Haberhauer², Matthias Epple¹

¹ Inorganic Chemistry and Center of Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitaetsstr. 5-7, 45117 Essen ² Organic Chemistry, University of Duisburg-Essen, Universitaetsstr. 5-7, 45117 Essen

E-Mail: kathrin.kostka@uni-due.de

The interest in ultrasmall nanoparticles is steadily increasing due to their importance in various applications such as in biomedicine [1] or as catalysts [2]. By attaching different ligands, the properties of the nanoparticles can be specifically controlled. In addition, a chiral nature of such nanoparticles and suitable analytical methods for that property are of great interest [3].

The surface of ultrasmall gold nanoparticles (usAu-NPs) can be covalently functionalized with chiral amino acids, such as cysteine, in an attempt to change the nature of the gold core. To investigate the chirality of the gold core, *L*-cysteine and *D*-cysteine functionalized ultrasmall gold nanoparticles (Au-*L*-Cys and Au-*D*-Cys) were prepared by reducing the gold precursor tetrachlorogoldic acid (HAuCl₄) with sodium borohydride (NaBH₄) under mild conditions at room temperature. By ligand exchange with the achiral ligand mercaptoacetic acid (Au-Mes), and subsequent exchange with *D*-cysteine and *L*-cysteine ligands, respectively, the chirality of the gold nanoparticle can be studied after each synthetic step.

For the complete characterization of the functionalized usAu-NPs (before and after ligand exchange), a colloidal-chemical analysis was performed by disc centrifugal sedimentation (DCS), NMR spectroscopy, and UV-Vis spectroscopy. Circular dichroism (CD) spectroscopy was applied to investigate the chirality of the gold nanoparticles.



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38: Competing Processes as Quality Limitation: New Insights into Microscopic Growth Mechanism of Hexagonal Boron Nitride on Ir(111)

Karim M. Omambac¹, <u>Marko A. Kriegel¹</u>, Marin Petrovic², Birk Finke¹, Christian Brand¹, Frank-J. Meyer zu Heringdorf^{1,3} and Michael Horn-von Hoegen¹

 ¹ Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany
 ² Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Bijenička 46, 10000 Zagreb, Croatia
 ³ Interdisciplinary Center for Analytics on the Nanoscale (ICAN), Lotharstraße 1, 47057

Duisburg, Germany

E-Mail: marko.kriegel@uni-due.de

Despite the tremendous research efforts targeting industrial growth of two-dimensional hexagonal boron nitride (hBN), especially on transition metal surfaces, until today no growth recipe was developed, promising large domain sizes, homogeneous lattice constants and a matching orientation of layer and substrate. We studied CVD grown hBN on Ir(111) with borazine as precursor and found two competing processes governing the quality of the hBN layer on a microscopic scale: kinetic limitations after catalytic borazine decomposition and dissociation of B3N3 rings with loss of nitrogen followed by disintegration of the grown layer. The counteracting interplay of all processes sets a fundamental limit to the achievable quality, due to defect-creation upon dissociation of the rings. We combined results from spot profile analyzing low energy electron diffraction (SPA-LEED), allowing us to determine the distribution of domain orientations from a representative surface area, and low energy electron microscopy (LEEM), for the measure of domain density [1]. Our understanding of the microscopic processes during hBN growth further enable us to selectively tune the growing material, hBN or 2D Boron (Borophene), representing a potential pathway to lateral heterostructures.

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39: Scalable light emitting and light sensing devices based on 2D materials and 2D heterostructures

<u>T. Kümmell</u>¹, Y. Beckmann¹, H. Myja¹, D. Andrzejewski¹, U. Hutten¹, A. Grundmann², H. Kalisch², M. Heuken^{2,3}, A. Vescan², K. Musselman⁴, I. Goldthorpe⁵, G. Bacher¹

¹Werkstoffe der Elektrotechnik & CENIDE, University of Duisburg-Essen, Germany ²Compound Semiconductor Technology, RWTH Aachen University, Germany ³AIXTRON SE, Herzogenrath, Germany

⁴ Department of Mechanical & Mechatronics Engineering & WIN, University of Waterloo, Canada

⁵ Department of Electrical & Computer Engineering & WIN, University of Waterloo, Canada

E-Mail: tilmar.kuemmell@uni-due.de

Transition metal dichalcogenides (TMDCs) have emerged as highly promising semiconducting materials for ultrathin optoelectronic devices. However, actual device concepts are mainly based on mechanically exfoliated crystals, resulting in only µm-sized prototypes. Metalorganic chemical vapor deposition (MOCVD) has proven to allow for the fabrication of TMDCs and TMDC heterostructures up to wafer-scale. In our contribution, we present architectures for light emitting and light sensing devices with active areas in the mm² range that are based on 2D semiconductor layers grown by MOCVD.

For light emitting devices (LEDs), we use a vertical p-n layout, which is scalable and reproducible. MOCVD grown WS₂ monolayers are embedded between organic and inorganic injection layers on the anode and the cathode side, respectively. LEDs with characteristic red luminescence with an area of several mm² and a turn on voltage as low as 2.5 V were fabricated on rigid [1,2] and flexible [3] substrates. By bending a flexible device, the emission can be tuned by more than 30 meV due to an in-plane strain-induced bandgap shift of the WS₂. The use of Ag nanowire networks as the cathode allows the fabrication of fully transparent LEDs with an average transmittance of about 60 % in the visible spectral range.

For light sensing devices, 2D material heterostructures are incorporated in order to achieve higher efficiencies or to provide additional functionality. We show that in photodetectors based on a heterostructure consisting of MoS_2 and WS_2 monolayers, a striking performance increase is obtained: Responsivity and gain of a WS_2/MoS_2 heterostructure photodetector are 5 orders of magnitude higher than in photodetectors based on single MoS_2 or WS_2 layers, respectively [4]. For $MoS_2/Graphene$ heterostructure photodetectors a methodology was developed for separating adsorbate effects from charge carrier separation at the heterostructure switches from p-type to n-type [5]. These findings open interesting perspectives for photodetectors that are sensitive to the environment.

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40: Fabrication and electrochemical characterization of 2D membranes

<u>Yossarian Liebsch¹</u>, Lukas Madauß¹, Jan Siebenborn¹, Vanina Cayón², Maria Eugenia Toimil Molares² and Marika Schleberger¹

> ¹ Universität Duisburg-Essen ² Material Research at GSI

E-Mail: yossarian.liebsch@uni-due.de

Two-dimensional (2D) materials have the potential to revolutionize industrial and technical processes such as water filtration, desalination, and energy storage due to their extremely thin nature. With a thickness of only a few angstroms, they have the potential to serve as highly efficient membranes, outperforming traditional membranes by orders of magnitude. Membranes play a critical role in many industrial and technical processes, making this potential breakthrough extremely promising. We created two types of 2D membranes using commercially available CVD-grown graphene and self-grown CVD MoS₂, respectively. To generate nanopores, we transferred the 2D materials onto a 3 μ m micropore and then plasma etched the graphene or irradiated the MoS₂ with highly charged ions. We analyzed the membranes using Raman and photoluminescence spectroscopy to study their doping, stress, and defect density. We also performed electrochemical measurements using a custom-built membrane potential measurement stand. The measured graphene membrane potentials showed good agreement with the Theorell-Meyer-Sievers Theory, but we were unable to measure the potential for the MoS₂ membranes. Our future experiments with this electrochemical cell will explore the relationship between pore creation mechanisms and membrane properties such as pore size, pore chemistry, and surface charge density.



41: The Influence of Ions Present and pH of the Electrolyte on the Electrochemical Oxygen Reduction to Hydrogen peroxide in Carbon Electrodes

Ricardo Martínez-Hincapié, Viktor Čolić

Electrochemistry for Energy Conversion, Max Planck Institute for Chemical Energy Conversion

E-Mail: ricardo.martinez-hincapie@cec.mpg.de

Hydrogen peroxide (H_2O_2) is an important chemical commodity used in a wide variety of industrial processes, including waste treatment, pulp and textile bleaching, and chemical synthesis [1]. Currently, 95% of the world demand for H_2O_2 is met via the centralized and energy intensive anthraquinone oxidation process [1]. On the other hand, the electrosynthesis of H_2O_2 is a decentralized and sustainable route where only electricity, H_2O , and O_2 are required [2]. Achieving high selectivity for oxygen reduction via the two-electron pathway is key for the development of sustainable approaches for the on-site electrochemical production of H_2O_2 . However, the factors controlling the activity and selectivity at the electrode/electrolyte interphase are not well understood [3].

In this work, a glassy carbon electrode was used as a model of carbon-based materials in contact with alkali cations-containing acidic/alkaline solutions. The results allow us to obtain a more detailed picture of the carbon/electrolyte electrical double layer. The activity and selectivity of different interphases are measured with a rotating ring-disk electrode setup. Careful cleaning procedures and the use of gold instead of platinum as material for the ring electrode assure the quality of the results. This information could contribute to the rational development of electrode/electrolyte interphases to improve the activity and selectivity in onsite electrochemical H_2O_2 production when carbon-based electrodes are used.

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42: Multiplex immunogold staining of cancer-related proteins on Tokuyasu cell sections

Simon Mennicken¹, Louisa Waasmann¹, Sylvia Voortmann², Bernd Walkenfort² and Sebastian Schlücker¹

¹ Physical Chemistry I, Department of Chemistry and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstr. 5, Essen 45141, Germany.
² Institute for experimental Immunology and Imaging, University Hospital Essen, Universitätsstr. 2, 45141 Essen, Germany

E-Mail: simon.mennicken@uni-due.de, sebastian.schluecker@uni-due.de

Multiplex immungold labeling on cell sections is a technique used in cancer research and diagnostics to detect multiple targets in cancer cells simultaneously.^[1] It involves the use of antibody functionalized gold nanoparticles targeted to specific cancer-associated proteins. The bioconjugated gold nanoparticles can be visualized using transmission electron microscopy, given that the technique provides a highly sensitive method for the detection and localization of target antigens on cells.

Here, we developed a staining protocol with gold nanoparticles functionalized with four different cancer-associated antibodies to detect four antigens on the cell membrane, the mitochondria, the cytoskeleton, and the cell nucleus simultaneously. Four types of gold nanoparticles (8 nm, 14 nm, 22 nm spheres and 18 nm rods) with small standard deviations (<10%) were synthesized (Fig. a). In order to verify the specificity of binding, each type of gold nanoparticle was functionalized with a different antibody (anti-HER2, anti-mitochondrial, anti-cytokeratin and anti ERCC1). Therefore, each nanoparticle-type marked a different antigen on within the cell (Fig. b).



Figure 3: (a) Goldnanospheres and goldnanorods used for multiplex immungold targeting. (b) Simultaneous immunogold staining of mitochondrial (green arrow), membrane (red arrow), filament (orange arrow), and nuclear (blue arrow) proteins on Tokuyasu cell sections of SkBr3 cancer cells.

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43: PECVD-grown graphene used as conductive transparent electrodes in gallium nitride-based UV LEDs

U. Kaya, J. Meier, H. Zhang, W. Mertin, G. Bacher

University of Duisburg-Essen & CENIDE, Bismarckstr. 81, 47057 Duisburg, Germany

E-Mail: wolfgang.mertin@uni-due.de

The growing world population, combined with constantly rising temperatures due to climate change, is leading to an increasing spread of diseases. Preventing this spread is essential. An important measure to this end is the use of effective disinfection processes with deepultraviolet light (UVC, emission range 280 nm to 200 nm). Therefore, UVC light-emitting diodes (LEDs) based on $Al_xGa_{1-x}N$ are becoming increasingly important. However, these LEDs still have a very low performance. One of the reasons is the poor conductivity of the p- $Al_xGa_{1-x}N$ layer, which hinders sufficient lateral current distribution on the p-side of the LED [1]. Graphene simultaneously exhibits high electrical conductivity and high optical transparency in the UV spectral region and can therefore serve as a current-spreading layer (TCSL) [2,3]. However, device-compatible low-temperature integration of graphene in UVC LEDs has not yet been demonstrated.

Here we present the successful direct growth of a graphene layer on top of the p-Al_xGa_{1-x}N cladding layer in an UVC-LED. For the growth, we employ a plasma-enhanced (PE) Chemical Vapor Deposition (CVD) process with a methane/nitrogen mixture at temperatures as low as 670°C, expanding our previous work on GaN [3]. Optimizing gas mixture ratio, growth temperature and growth time, we obtained graphene with Raman intensity ratios of I_D/I_G ≈ 1.6 and I_{2D}/I_G ≈ 1.4, respectively, which is the best published value for direct grown graphene on p-Al_xGa_{1-x}N. The optical transparency of the as-grown graphene exceeds 90% in a spectral range from 270 nm to 800 nm. We achieved a sheet resistance of around 5 kΩ/sq. Our UVC-LED with graphene as a TCSL shows a diode-like *I-V* behavior with a current density of approximately 0.1 mA/cm² at 4 V and 0.23 mA/cm² at 5 V, respectively. The emission maximum of the LED is at 267.5 nm, and a distinct current spreading effect is observed.

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44: Iontronic memories based on ionic redox systems

Elalyaa Mohamed¹, Sabine Josten¹, Frank Marlow^{1,2}

¹ Max Planck Institute für Kohlenforschung ² Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg 47057, Germany

E-Mail: mohamed@mpi-muelheim.mpg.de

lontronics is a concept of using ions to transmit, store or generate signal. As ions are the language of nature and electrons are the language of man-made information processing, connecting both may lead to more understanding of nature as well as to new computational systems which might be called neuromorphic. In the last decade, many iontronic devices were invented and studied. However, developing of iontronics requires the invention of more flexible devices. In our lab we developed a purely ionic voltage effect soft triode (IVEST) based on interfacial ion adsorption and redox oxidizer depletion¹. The IVEST was built with no need of sophisticated or expensive materials. This device is an electrochemical micro-cell, which consists of a top electrode and two bottom electrodes. It has a memory effects in the electrical resistance lasting for up to 6 h. These values were achieved by tuning an electrode interface, the electrolyte and diffusion properties. The depletion of ions in the device plays the biggest role in the memory mechanism. With a well-defined measurement protocols the results are more reproducible and the memory contrast reached 1.8. The IVEST might be promising for neuromorphic applications.

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45: Measurements of gas-phase iron species using advanced laserspectroscopy tools

Sheikh Ahmed Mujaddadi¹, Peter Fjodorow¹, Matthieu R. Lalanne², Mustapha Fikri¹, Jürgen Herzler¹, Igor Rahinov², Christof Schulz¹

¹ Institute for Energy and Materials Processes – Reactive Fluids, Center for Nanointegration, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany ² Department of Natural Sciences, The Open University of Israel, 4353701 Raanana,

Israel E-Mail: sheikhahmed.mujaddadi@uni-due.de

Gas-phase synthesis at high-temperature is a preferred method for generating nanoparticles with desired properties. Understanding the kinetics of these processes is crucial for optimizing the synthesis conditions and achieving the desired properties of the final product. Iron oxide nanoparticles are of practical interest, but their synthesis requires a detailed understanding of the gas-phase reactions, nucleation, and coagulation that govern their formulation [1]. FeO is a key gas-phase species that acts as a precursor for larger species, and the measurements are essential for quantifying its number density and understanding the formation of iron oxide particles in flames.

Spectroscopy provides information about the fate of gas-phase species, their concentration, and reaction rates throughout the synthesis process. Such quantitative measurements are necessary for understanding the details of the mechanisms. For determination of absolute concentrations, absorption cross-section data are needed. Intracavity absorption spectroscopy (ICAS) is a promising technique that can provide highly sensitive spectroscopic analysis for detecting low concentrations of gas-phase species [2].

This study utilized dye-laser-based ICAS to measure the absolute absorption cross-sections of FeO in shock-heated $Fe(CO)_5/O_2/Ar$ mixtures. Atomic resonance absorption spectroscopy (ARAS) was simultaneously used to measure Fe-concentration. ICAS, combined with ARAS, provides a powerful diagnostic tool for studying gas-phase species and their reactions, even in complex environments like plasma or flames.

In shock tubes, the simultaneous measurements of time-dependent Fe and FeO absorption of $Fe(CO)_5/O_2/Ar$ mixtures at high temperatures allow the determination of FeO concentrations (corresponding to Fe consumption) and thus the calculation of absorption cross-section data for FeO. This data can be used to study the more complex kinetics of the Fe/O_2 system at lower temperatures, where both Fe + O_2 reaction channels (Fe+O₂+M <=> FeO₂+M and Fe+O₂ <<=> FeO+O), as well as reactions in the incident shock waves, must be considered.

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46: Detailed Investigation of the Reaction Kinetics of Iron Oxide Synthesis

<u>Monika Nanjaiah¹</u>, Patrick Wollny¹, Piotr Cwiek¹, Matthieu R. Lalanne³, Sascha Apazeller², Christof Schulz², Igor Rahinov³, Andreas Kemp^{1,4}, Irenaeus Wlokas^{1,4}

¹ EMPI, Institute of Energy and Materials Processes – Fluid Dynamics, University of Duisburg-Essen, Duisburg, Germany

² EMPI, Institute of Energy and Materials Processes – Reactive Fluids, University of Duisburg-Essen, Duisburg, Germany

³ Department of Natural Sciences, The Open University of Israel, Raanana, Israel ⁴ CENIDE, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Duisburg, Germany

E-Mail: monika.nanjaiah@uni-due.de

Flame spray pyrolysis is one of the promising methods to produce metal oxide nanoparticles in a cost and material-effective way [1]. Recently, the fabrication of transition metal compound based nanomaterials via flame synthesis is gaining steadily increasing attention due to cost-effectiveness, purity, continuous production, scalability, and accessibility of metastable compounds [2]. Iron oxide nanoparticles are one of the most studied materials due to their wide range of applications [3, 4]. Understanding the gas-phase reaction kinetics plays a crucial role in the process modelling, control, and production of nanomaterials with desired functionalities.

In this work, iron pentacarbonyl (Fe(CO)₅), and iron(III) nitrate nonahydrate (Fe(NO₃)₃.9H₂O) precursor systems are investigated using separate low-pressure burner configurations. Gasphase iron pentacarbonyl doped flames were used to validate the developed iron mechanism and study the impact of gas-phase iron compounds on the flame structure, further a single-particle Monte-Carlo simulation provided insights into the temperature history of the incipient particles complementing the experimental data. Using the developed iron reaction mechanism as the basis, iron nitrate/1 -butanol aerosol doped flames were investigated to study the impact of the precursor on flame chemistry. Additionally, the particle dynamics of the system were studied. Overall, this work presents an overview of the reaction kinetics of iron oxide forming flames, their impact on the flame chemistry, particle dynamics and the temperature history of the incipient particle, which drives us toward the predictive synthesis of nanomaterials with tailored functionalities.

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47: Tailoring pore size and catalytic activity in cobalt iron layered double hydroxides and spinels by microemulsion-assisted pHcontrolled co-precipitation

<u>Anna Rabe¹</u>, Maximilian Jaugstetter², Felix Hiege², Nicolas Cosanne³, Klaus Friedel Ortega³, Julia Linnemann², Joachim Landers¹, Soma Salamon¹, Kristina Tschulik², Malte Behrens³, Heiko Wende¹

> ¹ University of Duisburg-Essen, Department of Physics ² Ruhr University Bochum. Analytical Chemistry II ³ Christian-Albrechts-University Kiel, Institute for Inorganic Chemistry

> > E-Mail: anna.rabe@uni-due.de

Conventional aqueous co-precipitation of cobalt iron containing layered double hydroxides (LDHs) and spinels, which are promising catalysts for the electrochemical oxygen evolution reaction (OER), is well-established.[1,2] Towards the development of catalysts with improved activity and stability it is pivotal to be able to control and tune mesostructural features to allow the investigation of structure-activity relationships.

We herein established the computer-controlled microemulsion-assisted co-precipitation (MACP) at constant pH. The as-prepared LDHs and spinels derived from subsequent thermal decomposition were compared to samples from conventional co-precipitation. With MACP the particle growth is limited within the micelles and through variation of the constant pH during synthesis the pore size of the as-prepared catalysts is controlled, generating materials suited for the systematic investigation of confinement effects during OER. Detailed electrochemical investigations were performed and a threshold pore size at which overpotential increased significantly was identified. In this context, electrochemical impedance spectroscopy (EIS) indicated a change in OER mechanism, involving the oxygen release step. It is assumed that in smaller pores the critical radius for gas bubble formation is not met. Therefore, the pore outlet may not be blocked, affecting the local oxygen concentrations and leading to the smaller charge-transfer resistances observed at medium frequencies.[3]

To learn more about the ion occupation in the as-prepared samples, Mössbauer spectroscopy and magnetometry were performed with the prospect of designing an *operando* Mössbauer cell, to follow the structure of iron containing catalysts during electrochemical reactions.

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48: Role of surface termination and orientation on the activity of CoFe₂O₄(001) and (100) surfaces for water oxidation

Shohreh Rafiezadeh¹, Rossitza Pentcheva¹

¹ Department of Physics and Center for Nano integration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg

E-Mail: shohreh.rafiezadeh@uni-due.de

The inverse spinel $CoFe_2O_4$ plays an important role as an anode material for the electrochemical water splitting. This requires a fundamental understanding of the effect of surface termination and orientation on the OER activity. While the (001) facet of $CoFe_2O_4$ contains alternating layers of octahedral Co and Fe, the (100) surface comprises mixed Co and Fe layers. Here, by employing density functional theory calculations with an onsite Hubbard *U* term (DFT+*U*) we explore the OER performance of $CoFe_2O_4(100)$ and iron-rich (001)_{Fe} surfaces and compare to the cobalt-rich (001)_{Co} surface [1].

Co reaction sites at the A-layer termination which features an additional tetrahedral Fe-layer are found to have the lowest overpotentials: the lowest value is 0.20 V at the mixed Co-Fe $(100)_{Co&Fe}$ surface, followed by 0.38 V is found at the Co-rich (001) surface. The overpotentials of Fe reaction sites are above 0.44 V. This reduction of overpotential correlates with a bulk-like Co²⁺ oxidation state at the A-layer and a stabilization of the *OOH intermediate due to hydrogen bonding to neighboring sites. Further investigation of the density of states indicates that a stronger deviation of magnetic moment and oxidation state of both Co and Fe cations during OER from bulk results in a lower activity.

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49: Compact Setup for the Electrochemical Deposition and Alloying of Metals in a Controlled Atmosphere

Ali Raza Khan¹, Viktor Čolić^{1,2}

¹ Electrochemistry for Energy Conversion, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr, Germany ² Center for Nanointegration Duisburg-Essen (CENIDE), Duisburg, 47057, Germany

E-Mail: ali-raza.khan@cec.mpg.de

A new setup is presented to perform the electrochemical deposition, thermal treatment, and evaluation of the electrochemical performance of novel electrocatalysts for important reactions, including the oxygen reduction reaction (ORR), oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in a controlled environment without exposing the electrode to the laboratory atmosphere. Considerable attention has been paid to model singlecrystal surfaces in electrocatalysis, particularly to improve the understanding of structureactivity relationships. Determining the structure and dynamics of metal on solid surfaces is both fundamental and technologically important. The electrocatalytic properties of metals deposited at submonolayer coverage formed by underpotential and bulk deposition (UPD) can vary significantly from those of bulk materials[1]. After deposition (UPD), the electrode will be thermally annealed to make surface alloys (SAs) or near-surface alloys (NSAs)[2]. The surface alloy properties can be tailored by controlling the temperature and reactive gas environment. A digital infrared thermometer will be used to monitor the temperature in real-time and protocol the heating and cooling. The working electrode (WE) can be moved vertically up for annealing with an induction heater without removing from the cell in the control environment. A second compartment attached to the cell will be used to replace the precondition electrolyte. A dummy Pt wire parallel to the WE will be used to keep the WE potential under control during electrolyte replacement. By using this setup, we will synthesize Pt-Cu-Co, Pt-Cu-Ni SAs, and NSAs and examine their electrocatalytic properties. The electrocatalytic performance of the catalyst will be investigated using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), chronoamperometry, and other electrochemical techniques. The method will be coupled with an electrochemical quartz crystal microbalance (EQCM) for the quantification of deposited metals. To complement the electrochemical techniques, electrode surface characterization will be done with the help of different surface science techniques such as energy-dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS), and X-Rays Diffraction (XRD).



Figure: a) Cyclic Voltammogram of Pt Poly Electrode B) Schematic drawing of the cell



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50: Investigating the Absorption Properties Of Metal Nanoparticle Aggregates During Time-Resolved Laser-Induced Incandescense

<u>Stephen Robinson-Enebeli</u>^{1,2}, Christof Schulz², Kyle J. Daun¹ ¹ Department of Mechanical and Mechatronics Engineering, University of Waterloo, 200, University Ave W, Waterloo, ON, Canada ² EMPI, Institute for Energy and Materials Processes – Reactive Fluids, and CENIDE, Center for Nanointegration Duisburg Essen, University of Duisburg-Essen, 47048, Duisburg, Germany

E-Mail: stephen.robinson-enebeli@uwaterloo.ca

Metal nanoparticles play important roles in many disciplines, e.g., for catalysis or as materials with targeted magnetic properties. Gas-phase nanoparticle synthesis is a promising route to meet the increasing demand for metal nanoparticles and, consequently, there is a need to reliably characterize nanoparticles for their size and concentration. Time-resolved laser-induced incandescence (TiRe-LII) allows for in situ measurements that can provide both temporal and spatial information on aerosolized nanoparticles. The technique involves heating up the gas-borne nanoparticles with a nanosecond laser pulse, commonly at 1064 nm, and measuring their incandescence at different wavelengths as they cool down. A measurement model comprised of spectroscopic and heat transfer submodels is regressed to the data to infer quantities such as the size distribution of the nanoparticles, their concentration, and the efficiency with which they exchange energy with the surrounding gas [1].

Analyzing time-resolved laser-induced incandescence (TiRe-LII) data from metal nanoparticle aerosols requires a detailed understanding of their absorption and emission characteristics. In particular, the incomplete understanding of the laser –nanoparticle interaction during laser heating as well as the impact of laser-induced morphological changes on the absorption cross-section are possible sources of reported anomalies, such as excessive absorption (where the peak experimental temperatures reached by laser-heated nanoparticles exceed predicted values) and anomalous cooling (where nanoparticles cool faster immediately after reaching their peak temperature than can be explained by current heat transfer models) that are yet to be fully explained by the models [2–4].

In this work, we investigate the effects of nonuniform absorption within metal nanoparticle aggregates, aggregate orientation, and sintering of primary particles on the absorption properties of aggregates used in TiRe-LII models of metal aerosols. The multi-sphere T-matrix method was used to compute the absorption properties of aggregates with point contact between primary particles and the discrete dipole approximation method was used when primary particles overlap. It was found that absorption non-uniformities within aggregates increase with increasing aggregate sizes, and may contribute to excessive absorption and anomalous cooling effects. For the aggregates considered, the total absorption cross -section depends weakly on orientation. It was found that primary particle overlap of about 20–30 %, resulting from partial sintering, can enhance the absorption cross -section of the aggregate.



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51: Optoelectronic properties of Janus MoSSe and nonstoichiometric MoS_{2(1-x)}Se_{2x}

<u>Jennifer Schmeink¹</u>, Vladislav Musytschuk¹, Nicolas Hille¹, Erik Pollmann¹, Peter Kratzer¹, and Marika Schleberger¹

¹ Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

E-Mail: jennifer.schmeink@uni-due.de

Classic transition metal dichalcogenides (TMDCs) are widely studied for their varied properties. They are the prime subject for all types of (opto-)electronic components. Even more so since TMDCs belong to the group of van-der-Waals-materials, which can readily be thinned down to a single molecular layer. This molecular layer consists of a layer of transition metal atoms (M = Mo, W, V, Sn...), sandwiched in between two layers of chalcogen atoms (X = S, Se, Te), which gives it the typical MX₂ structure.

In 2017 a new type of TMDC was fabricated for the first time. This material consists like before of a layer of transition metal atoms sandwiched between two layers of chalcogen atoms, however the top and bottom layer consist of two different types of chalcogen atoms (X,Y = S, Se, Te; X \neq Y). The structure of this new material corresponds to XMY (see fig. 1). These materials exhibit new properties facilitated by the structural and electronic break of symmetry in the out-of-plane direction. Theoretical predictions show interesting properties such as: an intrinsic dipole moment, in- and out-of-plane piezoelectricity, second harmonic generation and a large Rashba-effect.



Fig. 1: Structure of a single molecular layer of a Janus-type TMDC in a) top view and b) side view. The red and yellow spheres represent the two different chalcogen atoms, while the magenta spheres constitute the transition metal atoms.

The fabrication of a Janus monolayer commonly starts off from a base TMDC's monolayer which top-most layer is selectively substituted with another kind of chalcogen atoms. However, if the substitution is partial, the resulting material resembles more an alloy than a Janus-type structure. These in-between materials show their own interesting features, as they allow for example a fluid optical bad-gap tuning from that of MoSe₂ at 1.54 eV over 1.70 eV for MoSSe up to 1.84 eV of MoS₂.

Recently we were able to synthezise MoSSe Janus monolayers [1]. We are happy to show our recent progress in characterizing this new material's properties. Moreover, we want to explore the monolayer $MoS_{2(1-x)}Se_{2x}$ ($0 \le x \le 1$) in-between structures and how we can learn from their features about our Janus structures.



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52: Time-resolved UV-visible absorption spectroscopy of young soot particles during toluene pyrolysis in a shock-tube

Can Shao, Mustapha Fikri, Torsten Endres, Christof Schulz

Institute for Energy and Materials Processes – Reactive Fluids, University of Duisburg Essen

E-Mail: can.shao@uni-due.de

Although soot particle formation in the combustion process has been studied for decades, mysteries remain especially in the transition from gas-phase molecules to carbon clusters and initial particles. There are three hypotheses for the key inception mechanism: 1) Combination of two-dimensional polycyclic aromatic hydrocarbons (PAHs) with fullerene-like structure; 2) Physical coalescence of PAHs into stacked clusters, called physical dimerization or physical inception, and 3) Chemical coalescence of PAHs into cross-linked, three-dimensional structures, named chemical dimerization or chemical inception. Unfortunately, there are no solid arguments to support each hypothesis, especially when accounting for the prevailing temperature. In this work, the time-resolved absorption spectroscopy measurement was conducted on shock-heated reactive toluene/argon mixtures for observing the UV-visible absorption properties of young soot particles and their precursors throughout their transition from gas-phase species to incipient particles. The transmitted light that carries the absorption information from the species inside the shock tube was recorded temporally and spectrally resolved using the setup as shown in Figure. 1. A laser-driven light source was used as a broadband UV-visible light source. After collimation, the light passed through quartz windows mounted in the sidewall of the shock tube which is located 30 mm upstream of the end wall. After passing the exit window, the transmitted light was focused by a quartz lens onto the entrance slit f an imaging spectrometer. The spectrometer was coupled to a UV-sensitive backilluminated EMCCD camera. After triggering the camera with the signal from the pressure transducer that recorded the passage of the incident shock wave, reaction-time-resolved absorption spectra were recorded. Post-reflected-shock temperatures varied from 1200 to 2800 K. From the results, the absorption properties vary with temperature, which indicates the different inception pathways. Understanding the absorption properties of these species will-in addition to clarifying the particle inception mechanism.



Keywords: UV-visible absorption, shock tube, pyrolysis, soot, inception







53: Time-resolved X-ray absorption spectroscopy at a Fe(II) spincrossover molecule at the European XFEL

L. Spieker¹, G. Kämmerer¹, T. Lojewski¹, L. Mercadier², A.Scherz², L. le Guyader², M. Teichmann², R. Carley², G. Mercurio², N. Gerasimova², N. van Kuiken², C. Carnian², D. Hickin², S. K. Kuppusamy³, M. Ruben^{3,4}, J. Grunwald⁵, F. Tuczek⁵, K. Ollefs¹, C. Schmitz-Antoniak⁶, P. Kratzer¹, K. Sokolowoski-Tinten¹, M. Gruber¹, A. Eschenlohr¹, U. Bovensiepen¹, H. Wende¹

 ¹ Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany
² European XFEL, 22869 Schenefeld, Germany
³ Institute for Quantum Materials and Technologies (IQMT), Karlsruhe Institute for Technology (KIT), 76344 Eggstein-Leopoldshafen, Germany
⁴ Centre Européen de Sciences Quantiques (CESQ), Institut de Sciene et d'Ingénierie Supramoléculaires (ISIS), 67083 Strasbourg Cedex, France
⁵ Institute for anorganic chemistry, Christian-Albrechts-University Kiel, 24098 Kiel, Germany
⁶ Faculty of Engineering and Natural Sciences, Technical University of Applied Science Wildau, 15745 Wildau, Germany

E-Mail: lea.spieker@uni-due.de

Spin-crossover complexes with a bistable spin-state switching from a low-spin to a high-spin state in the room temperature regime, influenced by external stimuli such as light or temperature, are desirable for future applications, e.g., molecular switches. Time-resolved X-ray absorption spectroscopy (tr-XAS) allows the analysis of the spin-states after an optical pump event on the femtosecond timescale. At the SCS instrument at the European XFEL [1], we measured tr-XAS of a Fe(II) spin-crossover thin-film with unprecedented data quality. This allows the resolution of spectral features that can be assigned to the low-spin and high-spin states and the observation of the occupation dynamics. Therefore, we can investigate the ultrafast femtosecond dynamics of the spin-state switching process and possible cooperative effects.

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54: How does the immune system react on albumin-derived perfluorocarbon-based artificial oxygen carriers (A – AOCs)?

LM. Tchuendem¹, Felix Bos¹, N. Uhde¹, Holger Jastrow^{2, 3}, KB. Ferenz^{1, 4}

 ¹ University of Duisburg-Essen, University Hospital Essen, Institute of Physiology, Essen, Germany
² Institute of Anatomy, University of Duisburg-Essen, University Hospital Essen, Hufelandstr. 55, Essen, Germany
³ Imaging Center Essen, Electron Microscopy Unit, University of Duisburg-Essen, Hufelandstr. 55, Essen, Germany
⁴ CENIDE, University of Duisburg-Essen, Duisburg, Germany

E-Mail: linda.tchuendem@uk-essen.de

Artificial oxygen carriers (AOC) improve tissue oxygenation and thus comprise a possible alternative to infusion of allogenic red blood cells¹ in case of a lack of blood donors, of emergency or if allogenic blood is no option for religious reasons. Albumin-derived perfluorocarbon-based artificial oxygen carriers (A-AOCs) are applied by intravenous injection^{1,2}. In the body, A-AOCs are, however, detected and processed by immune cells, among which macrophages are of major importance. We analyzed the response of two different types of murine macrophages, i.e., bone marrow derived macrophages (BMDM) and J774 cells (which comprise a cultured murine macrophage cell line) exposed to different concentrations of A –AOCs. In case of activation of the immune system, the concentration of specific cytokines and the expression of selected immunologically relevant genes should increase.

BMDM and J774 macrophages were treated with pure cell culture medium or medium with 5% bovine serum albumin which both do not activate the immune system, 2-10% of A-AOCs with 5% bovine serum albumin (potential activation) or 1 μ g/ml lipopolysaccharide (LPS, strong activation) at 21% O₂ and 5% CO₂ for 24h. To analyze the influence of A -AOCs on release of cytokines, we measured the concentration of tumor necrosis factor alpha (TNF alpha) and interleukin-1alpha (IL-1alpha) by ELISA in the cell culture supernatant. Further, we quantified mRNA expression of selected immunologically relevant genes (*Tnf alpha* and *II-1alpha*) by quantitative PCR.

The uptake of A –AOCs into BMDM and J774 macrophages ($5x10^5$ cells/ml) was visualized at 488 and 643 nm using confocal microscopy. For this, cells were incubated with 100 µg/ml TRITC-Concavalin A for 30 min followed by 4% of FITC-labelled A –AOCs for 30 min or 2 h. For a more detailed analysis we verified this by transmission electron microscopy: after incubation with 1% OsO₄ in PHEM buffer and contrastation with 1% uranyl acetate 55 µm-ultrathin sections were cut from Epon embedded samples. Sections were mounted on 200 MESH copper grids and micrographed by a TemCam-F416 on a Jeol JEM 1400 Plus TEM.

ELISA measurements revealed an activation of the immune system only for BMDM and J774 macrophages treated with LPS, a potent activator of macrophages. In addition, quantitative PCR demonstrated a low RNA expression of the selected immunologically relevant genes *Tnf alpha* and *II–1alpha*. Both, confocal and electron microscopy visualised an uptake of A –AOCs by BMDM and J774 macrophages already after 30 min, which further increased after 2 h of incubation.

In conclusion, our results demonstrate that, although BMDM and J774 macrophages engulf A –AOCs, the immune system is not activated by their presence.





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55: Mixed metal oxides as oxygen carrier for chemical looping oxidative dehydrogenation of ethane

D. Zhang¹, X. Tian^{1,2,*}, M. Ding¹

¹ School of Power and Mechanical Engineering, Wuhan University, 430072 Wuhan, China ² Institute for Energy and Materials Processes – Reactive Fluids, University of Duisburg-Essen, 47078 Duisburg, Germany

E-Mail: xin.tian@uni-due.de

Chemical looping oxidative dehydrogenation (CL-ODH) of ethane offers a new strategy for ethylene production. In CL-ODH, an oxygen carrier (rather than pure O_2) is used to provide the oxygen required for ODH reactions, thus eliminates the energy-intensive air separation unit as well as safety hazards regarding to O_2 /ethane co-feeding. Undoubtedly, oxygen carrier with sufficient oxygen capacity and high selectivity towards ethylene is critical for CL-ODH of ethane.

However, achieving high ethylene selectivity as well as promising ethane conversion at relatively low-temperature (≤ 600 °C) in CL-ODH of ethane is still challenging. Herein, we show that Fe-Co dual-metal oxides supported HZSM-5 can be used as appropriate redox catalyst for low-temperature CL-ODH of ethane. By tuning the loading mass ratio of Fe: Co oxides on the HZSM-5 support, 87% ethylene selectivity and 23% ethane conversion can be attained at 600 °C and 4800 mL·h⁻¹·g⁻¹ with the best-performing sample, *i.e.*, 8Fe-2Co/HZ5(200). The stability of this sample was then assessed across 100 redox cycles, no obvious coking was observed within the entire test. Comparison test and physicochemical characterization results showed that both sample acidity and dual-metal oxides synergy are pivotal for ethane ODH to yield ethylene, in which dual-metal oxides are responsible for low-temperature ethane activation while proper amount of medium strength acidity is critical for ethylene selectivity as well as activity. In summary, the present work demonstrates the feasibility of using dual-metal oxides promoted HZSM-5 for low-temperature CL-ODH of ethane, and provides a facile way for redox catalyst design to balance sample activity and selectivity.

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56: Metalorganic-based Synthesis of thermoelectric (Bi_xSb_{x-1})₂Te₃ Nanoparticles

Charlotte van Halteren¹, Prof. Dr. Stephan Schulz¹

¹ University of Duisburg-Essen, Faculty of Inorganic Chemistry, Universitätsstraße 7, 45141 Essen

E-Mail: charlotte.van-halteren@uni-due.de

Thermoelectric (TE) generators are a promising technology to provide a solution to the energy crisis. TE generators consist of TE materials that can convert unused waste heat, such as that generated by car engines and industrial processes, into usable electrical energy via the Seebeck effect. However, the efficiency of energy conversion is limited by their thermal conductivity in addition to their desired electrical conductivity [1]. Although many efforts have been made to overcome these limitations, including nanostructuring and doping [2], the state-of-the-art materials still show relatively low conversion efficiency, which prevents widespread application [3]. This is often due to off-stoichiometric composition, oxidation, and contamination of the product by medium or organic impurities during fabrication. Therefore, it is of interest to open new synthetic routes for nanostructured phase-pure TE materials with excellent surface purity.

We herein present the successful synthesis of ternary $(Bi_xSb_{x-1})_2Te_3$ nanoparticles with x = 0.25, 0.5, 0.75 *via* the reaction of suitable metalorganic precursors. With the aim of optimizing the synthetic procedure the composition, phase-, and surface purity of the material was analyzed in detail.



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57: Parametric Studies of Agrowaste Particle Incorporation in Electroplated Ni and Electroless Ni-P Coatings for Improved Coating Properties

F. U. Whyte^{1, 2}, M. Abedini¹, S. Hanke¹

¹ Materials Science and Engineering, Institute for Metal Technologies, University of Duisburg-Essen

² Department of Metallurgical and Materials Engineering, Faculty of Engineering, University of Nigeria, Nsukka, Nigeria

E-Mail: favour.uboho.whyte@stud.uni-due.de

This study focuses on the effects of second phase particle incorporation in electrodeposited Ni and electroless Ni-P coatings on steel substrate. We propose cow bone ash micro and nanoparticle incorporation in the coatings with the aim of improving the morphological, mechanical, corrosion and wear properties. Cow bones are a waste product of stock farming, and could serve as a sustainable resource, if their suitability to produce strengthening particles for metal coatings can be proven. This project has started recently and the motivation, state of the art, outline of the research steps as well as first results of the particle manufacturing route will be presented.

Cow Bone Ash particles (CBAp) have been prepared from cow bone waste by washing, cleaning, drying and calcining at 800°C. The calcined bones were crushed, ground and sieved (63-75 μ m) to produce the microparticles. The nanoparticles will be produced by a green manufacturing process [1]. S235JR steel is the substrate, and it will be prepared using standard procedures (ASTM B322-99) [2]. Electroless and electro plating baths of both the pure and composite (with CBAp) coatings will be prepared with varying concentrations and different particle sizes of the CBAp. The effect of CBAp addition in the coatings will be studied by microscopic evaluation (SEM/EDS, optical microscopy), mechanical evaluation (microhardness), corrosion evaluation (tafel polarization and electrochemical impedance spectroscopy) and tribological evaluation (friction co-efficient, wear and surface roughness). Fatigue testing and tribo-corrosion testing will be used to monitor the coating failure pattern and the amount of stress it can withstand until failure.

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58: Development of MgAgSb-based thermoelectric generators

<u>Arthur Wieder^{1,2}</u>, Julia Camut¹, Amandine Duparchy¹, Aidan Cowley², Eckhard Müller^{1,3}, Johannes de Boor^{1,4}

 ¹ Institute of Materials Research, German Aerospace Centre, Cologne, D-51147, Germany ² European Astronaut Centre, European Space Agency (ESA), Cologne, D-51147, Germany ³ Justus Liebig University Giessen, Institute of Inorganic and Analytical Chemistry, Giessen, D-35392, Germany
⁴ University of Duisburg-Essen, Faculty of Engineering, Institute of Technology for Nanostructures (NST), Duisburg, D-47057, Germany

E-Mail: Arthur.Wieder@dlr.de

The ability of thermoelectric generators (TEGs) to convert heat into electricity via the solid state Seebeck effect makes them highly attractive. TEGs consist of a series of doped n- and p-type semiconducting elements that are connected electrically in series by metallic bridges. Radioisotope thermoelectric generators (RTGs) used for power supply during NASA deep-space missions have demonstrated the usefulness and reliability of TEGs for specific applications. Most of TEGs are based on bismuth and telluride, but their scarcity, environmental harmfulness and toxicity impede their use on a larger scale. The development of TEGs based on abundant and non-toxic elements is therefore a crucial challenge.

Recent works have shown TEGs reaching high conversion efficiency of around 8.5 % with new types tellurium-free materials: Mg-based materials where α -MgAgSb is used as p-type semiconductor and Mg₃Sb₂ as corresponding n-type semiconductor [1]. α -MgAgSb is a promising thermoelectric (TE) material. Its constituents are more abundant than tellurium, and the TE material shows good mechanical properties. A high figure of merit value zT = 1.34 at 561 K has been reported previously in the literature [2], zT being a dimensionless parameter evaluating thermoelectric performance of a material. Materials reaching a zT value ≥ 1 are considered very good thermoelectric materials.

We have for the first time successfully fabricated a prototype based on optimized p-type α -MgAgSb and n-type Mg₂(Si,Sn) ($zT_{max} = 1.4$ [3]) TE materials, addressing challenges like optimization of the respective materials, interface design, mechanical stability and integrity of the device. In doing so, we have substituted the slightly more performant, but less abundant, more toxic and less lightweight n-type Mg₃Sb₂.

The prototype TEG shows an efficiency of 6.3 % for $T_c = 300$ K and $T_h = 573$ K, and a power density up to 1 W/cm² with respect to the TE components cross-section. It is so far the first efficiency and power density results for a α -MgAgSb/Mg₂(Si,Sn)-based TEG and among the best for TEG for the mid-temperature range, surpassing commercially available TEGs.

In order to check for the reliability of the measurement and indicate room for improvement, model calculations on TEG performance using a continuum theoretical model were compared to measurement results. An improvement of the conversion efficiency up to 7.5 % can be expected if the interface design is further optimized.

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59: Simulation of phase images obtained by electron holography for three-dimensional spin-textures

Moritz Winterott^{1,2}, Samir Lounis^{1,2}

¹ Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany ² Faculty of Physics, University of Duisburg-Essen and CENIDE, 47053 Duisburg, Germany

E-Mail: m.winterott@fz-juelich.de

Three-dimensional (3D) spin-textures, similarly to their 2D counterpart (skyrmions), are attracting widespread interest, especially because of their potential application as magnetic bits for energy-efficient storage devices.

Thereby, a major challenge is their identification. Here we focus on electron holography, where phase images are reconstructed in order to recognize 3D spin-textures. The phase image consists of an electronic and a magnetic contribution, with the latter being assumed to emerge from the stray field, and thus should vanish for antiferromagnets, while the former is conjectured to be inert to the magnetic texture. Here we demonstrate that the electronic phase image carries non-trivial magnetic information induced by spin-mixing and spin-orbit mechanisms. We calculate and compare systematically the strength of both electronic and magnetic phase images employing the optimized forward model [1] and a tight-binding scheme combined with multiple-scattering theory. We explore the impact of spin-orbit interaction, exchange splitting and hopping.

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60: Preparation of Superhydrophobic POSS/PVDF Composite Membrane for Membrane Distillation

Libing Zheng^{1, 2}, Deyin Hou¹, Yuansong Wei¹, Mathias Ulbricht²

¹ Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China

² Lehrstuhl für Technische Chemie II, Universität Duisburg-Essen, 45141 Essen, Germany

E-Mail: libing.zheng@gast.uni-due.de

The ascending requirement of water reuse and the popularization of zero liquid discharge (ZLD) raise an urgent need for industrial wastewater treatment in both academic and industrial world [1]. Membrane distillation (MD) had been recognized as a potential ZLD technology, but the fouling and wetting were still two unsolved issues, fostering an enduring pursuit for welldesigned superhydrophobic membrane. In this work, a novel hierarchically-structured superhydrophobic membrane was prepared by grafting octavinyl-polyhedral oligomeric silsesquioxane (OVPOSS) onto polyvinylidene fluoride (PVDF) membrane via UV-induced thiol-ene click reaction after the hydroxylation and sulfhydrylation pretreatment. The strong covalent binding of olefinic double bond and sulfydryl group was obtained by successful introduction of -OH and -SH, by which the superhydrophobic surface was engineered with a higher roughness of more than 500 nm. For the fabricated superhydrophobic membrane with low sliding angle (about 7.5°), the maintaining of Cassie-Baxter state and the "slip effect" significantly mitigated membrane fouling and wetting, due to the retardation of the liquid invasion into the gas-solid interface [2]. It was found that scaling was the leading fouling for the commercial PVDF membrane, and the interaction between Ca²⁺ and carboxyl was the main organic fouling mechanism. While for the POSS/PVDF membrane, organic fouling via hydrophobic-hydrophobic interaction was the main membrane fouling and the scaling was significantly alleviated [3]. The fabricated POSS/PVDF composite membrane had significant superiority over commercial PVDF membrane because of the excellent anti-fouling and antiwetting properties, which showed promising potential in challenging wastewater treatment. Additionally, this work also offered a new and facile method for superhydrophobic membrane fabrication.

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List of Participants

Last Name	First Name	Faculty/Institution	Email Address
AbuAwwad	Nihad	Physics	n.abuawwad@fz-juelich.de
Aceves	Uriel	Physics	u.aceves@fz-juelich.de
Aguiar M. V. dos Santos	Beatriz	Engineering	beatriz.santos@ctn.tecnico.ulisboa. pt
Aldarawsheh	Amal	Physics	a.aldarawsheh@fz-juelich.de
Amin	Adil	Engineering	adil.amin@uni-due.de
Apazeller	Sascha	Engineering	sascha.apazeller@uni-due.de
Bacher	Gerd	Engineering	bacher.unidue@gmail.com
Baik	Seung-Jin	Engineering	seung.baik@uni-due.de
Barcikowski	Stephan	Chemistry	tc1.secretary@uni-due.de
Bendt	Georg	Chemistry	georg.bendt@uni-due.de
Böhm	Miriam	CENIDE	miriam.boehm@uni-due.de
BRANDAU	SVEN	Medicine	sven.brandau@uk-essen.de
Braun	Michael	Chemistry	michael.braun@uni-due.de
Breuer	Lars	Physics	lars.breuer@uni-due.de
Chatwani	Mohit	Engineering	mohit.chatwani@stud.uni-due.de
Cifuentes	Luis	Engineering	luis.cifuentes@uni-due.de
Colic	Viktor	MPI-CEC	viktor.colic@cec.mpg.de
Daniel	Leon	Physics	leon.daniel@uni-due.de
De	Sayantan	Biology	sayantan.de@uni-due.de
de Boor	Johannes	Engineering	johannes.deboor@dlr.de
Schleberger	Marika	Physics	marika.schleberger@uni-due.de
Duaprchy	Amandine	Engineering	amandine.duparchy@dlr.de
Dubey	Astita	Engineering	astita.dubey@uni-due.de
Ebertz	Felix	Engineering	felix.ebertz@uni-due.de
El Moussawi	Abbas	Engineering	abbas.moussawi@uni-due.de
Endres	Torsten	Engineering	torsten.endres@uni-due.de
Epple	Matthias	Chemistry	matthias.epple@uni-due.de
Eschenlohr	Andrea	Physics	andrea.eschenlohr@uni-due.de
Everschor- Sitte	Karin	Physics	karin.everschor-sitte@uni-due.de
Fainblat	Rachel	Engineering	rachel.fainblat-padua@uni-due.de
Feggeler	Thomas	University of California - Berkeley	tfeggeler@berkeley.edu
Feng	Huayang	Chemistry	huayang.feng@stud.uni-due.de
Ferenz	Katja	Medicine	katja.ferenz@uk-essen.de
Fikri	Mustapha	Engineering	mustapha.fikri@uni-due.de
Fischer	Lukas	Chemistry	lukas.fischer@uni-due.de
Fjodorow	Peter	Engineering	peter.fjodorow@uni-due.de
Foo	Cheau Tyan	Engineering	cheau.foo@stud.uni-due.de
Franke	Marion	NETZ	marion.franke@uni-due.de



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Last Name	First Name	Faculty/Institution	Email Address
Fu	Qingqing	Engineering	qingqing.fu@uni-due.de
Gabriel	Philipp	Chemistry	philipp.gabriel@uni-due.de
Galstyan	Anzhela	Chemistry	anzhela.galstyan@uni-due.de
Giese	Michael	Chemistry	michael.giese@uni-due.de
Giesler	Helene	Chemistry	helene.giesler@uni-due.de
Grishchuk	Ivan	Biology	ivan.grishchuk@stud.uni-due.de
Gruber	Manuel	Physics	manuel.gruber@uni-due.de
Gumbiowski	Nina	Chemistry	nina.gumbiowski@uni-due.de
Haag	Adrian	Chemistry	adrian.haag@uni-due.de
Hagemann	Ulrich	ICAN	ulrich.hagemann@uni-due.de
Häuser	Patrick	Engineering	patrick.haeuser@uni-due.de
Hausherr	Jacqueline	Chemistry	jacqueline.hausherr@freenet.de
Hechler	Michelle	Chemistry	michelle.hechler@uni-due.de
Heidelmann	Markus	Physics	markus.heidelmann@uni-due.de
Horn-von Hoegen	Michael	Physics	mhvh@uni-due.de
Hoster	Harry	Engineering	harry.hoster@uni-due.de
Kämmerer	Gerald	Physics	gerald.kaemmerer@uni-due.de
Karaminejad	Sadrollah	Engineering	sadrollah.karaminejad@uni-due.de
Karatzia	Aikaterini	Chemistry	aikaterini.karatzia@uni-due.de
Kharsah	Osamah	Physics	osamah.kharsah@uni-due.de
Kleszczynski	Stefan	Engineering	stefan.kleszczynski@uni-due.de
Koch	Christine	Physics	christine.koch@uni-due.de
Kodimana Ramakrishna n	Pradeep	Engineering	pradeep.kodimana- ramakrishnan@uni-due.de
Koehler	Tillmann	Physics	koehler@kofo.mpg.de
Kohse- Höinghaus	Katharina	Chemistry	kkh@uni-bielefeld.de
Kollwitz	Marvin	Chemistry	marvin.kollwitz@uni-due.de
Kostka	Kathrin	Chemistry	kathrin.kostka@uni-due.de
Kriegel	Marko	Physics	marko.kriegel@uni-due.de
Kümmell	Tilmar	Engineering	tilmar.kuemmell@uni-due.de
Landers	Joachim	Physics	joachim.landers@uni-due.de
Liebsch	Yossarian	Physics	yossarian.liebsch@uni-due.de
Lopez- Camara	Claudia-F.	Engineering	claudia-francisca.lopez@uni-due.de
Lounis	Samir	Physics	s.lounis@fz-juelich.de
Marlow	Frank	Physics	marlow@mpi-muelheim.mpg.de
Martinez Hincapie	Ricardo Alonso	MPI-CEC	ricardo.martinez- hincapie@cec.mpg.de
Mayer-Gall	Thomas	DTNW	mayer-gall@dtnw.de
Mennicken	Simon	Chemistry	simon.mennicken@uni-due.de



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Last Name	First Name	Faculty/Institution	Email Address
Mertin	Wolfgang	Engineering	wolfgang.mertin@uni-due.de
Meyer zu Heringdorf	Frank	Physics	meyerzh@uni-due.de
Mohamed	Elalyaa	Physics	mohamed@mpi-muelheim.mpg.de
Mohri	Khadijeh	Engineering	khadijeh.mohri@uni-due.de
Muckel	Franziska	Engineering	franziska.muckel@uni-due.de
Mujaddadi	Sheikh Ahmed	Engineering	sheikhahmed.mujaddadi@uni- due.de
Nanjaiah	Monika	Engineering	monika.nanjaiah@uni-due.de
Nocke	Fabian	Chemistry/Medicine	fabian.nocke@uk-essen.de
Ollefs	Katharina	Physics	katharina.ollefs@uni-due.de
Pentcheva	Rossitza	Physics	rossitza.pentcheva@uni-duisburg- essen.de
Peukert	Sebastian	Engineering	sebastian.peukert@uni-due.de
Pilaski	Moritz	ZBT	m.pilaski@zbt.de
Pratsinis	Sotiris	Engineering	pratsinis@ethz.ch
Prinz	Günther	Physics	guenther.prinz@uni-due.de
Rabe	Anna	Physics	anna.rabe@uni-due.de
Rafiezadeh	Shohreh	Physics	shohreh.rafiezadeh@uni-due.de
Raza Khan	Ali	Chemistry	ali-raza.khan@cec.mpg.de
Reichenberge r	Sven	Chemistry	sven.reichenberger@uni-due.de
Robinson- Enebeli	Stephen	Engineering	stephen.robinson-enebeli@uni- due.de
Roy Chaudhuri	Tista	Chemistry	r.tista@gmail.com
Schierning	Gabi	Engineering	gschierning@physik.uni- bielefeld.de
Schlögl	Robert	Chemistry	acsek@fhi-berlin.mpg.de
Schlücker	Sebastian	Chemistry	sebastian.schluecker@uni-due.de
Schmeink	Jennifer	Physics	jennifer.schmeink@uni-due.de
Schredelseke r	Theresa	CENIDE	theresa.schredelseker@uni-due.de
Schroer	Martin	Engineering	martin.schroer@uni-due.de
Schulz	Christof	Engineering	christof.schulz@uni-due.de
Schulz	Stephan	Chemistry	stephan.schulz@uni-due.de
Segets	Doris	Engineering	doris.segets@uni-due.de
Seidl	Karsten	Engineering	karsten.seidl@uni-due.de
Severit	Petra	ALTANA AG	petra.severit@altana.com
Shao	Can	Engineering	can.shao@uni-due.de
Soezeri	Selcuk	Physics	s.soezeri@fz-juelich.de
Sokolowski- Tinten	Klaus	Physics	klaus.sokolowski-tinten@uni- due.de
Spieker	Lea	Physics	lea.spieker@uni-due.de



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Last Name	First Name	Faculty/Institution	Email Address
Svejda	Jan Taro	Engineering	jan.svejda@uni-due.de
Sydow	Jan-Eric	Chemistry/Medicine	jan-eric.sydow@uk-essen.de
Szpak	Nikodem	Physics	nikodem.szpak@uni-due.de
Tchuendem	Linda	Chemistry	lindamarciale.tchuendem@uk- essen.de
Teckentrup	Tobias	CENIDE	tobias.teckentrup@uni-due.de
Tian	Xin	Engineering	xin.tian@uni-due.de
Vadala	Miriana	Engineering	miriana.vadala@uni-due.de
van Halteren	Charlotte	Chemistry	charlotte.van-halteren@uni-due.de
Vinayakumar	Vineetha	Engineering	vineetha.vinayakumar@uni-due.de
Voskuhl	Jens	Chemistry	jens.voskuhl@uni-due.de
Weimann	Nils	Engineering	nils.weimann@uni-due.de
Wende	Heiko	Physics	heiko.wende@uni-due.de
Whyte	Favour	Engineering	favour.otung@gmail.com
Wieder	Arthur	Engineering	arthur.wieder@dlr.de
Wiggers	Hartmut	Engineering	hartmut.wiggers@uni-due.de
Winterott	Moritz	Physics	m.winterott@fz-juelich.de
Wlokas	Irenäus	Engineering	i.wlokas@uni-due.de
Wöhrl	Nicolas	Physics	nicolas.woehrl@uni-due.de
Zheng	Libing	Chemistry	libing.zheng@gast.uni-due.de





General Information and Organization

Conference Language: English

Impulse Presentations: 15 + 5 minutes **Workshops:** 2 hours

Postdoc Talks: 12 + 3 minutes

Awards:

The best two posters from each Poster Session will be awarded a prize of each 100 Euro, so that in total there will be four prizes.

Jury members:

Poster Session I:	Seung-Jin Baik
	Pradeep Kodimana Ramakrishnan Katharina Ollefs

Poster Session II: Claudia-F. Lopez-Camara Manuel Gruber Vineetha Vinayakumar Jens Voskuhl

W-LAN name:KSH_GastW-LAN password:KSH-Online

Organization Team:

Daniela Bauer, Miriam Böhm, Sebastian Peukert, Tobias Teckentrup

Contact:

Dr. Tobias Teckentrup, Managing Director CENIDE Universität Duisburg-Essen Room NETZ 3.20, Campus Duisburg Tel.: 0203 37-98178, tobias.teckentrup@uni-due.de, www.cenide.de





Floor Plan:



2nd Floor







Walking and Talking Route:

