

Center for the Transformation of Chemistry

Transforming Chemistry Summit

Poster Program Book

[Jahnallee 59](#), Leipzig, Germany – 15–16 September 2026

<https://transforming-chemistry.org/en/summit2026/>

POSTER SESSION INFORMATION

Session Date & Time	Session 1: Sept 15, 2026 @ 1:00-2:00 pm Session 2: Sept 16, 2026 @ 12:30-1:30 pm
Location	Foyer Nord, Campus Jahnalle
Poster Board Size	120 x 150 cm portrait (A0, vertical)
Setup Window	Please set-up during registration time 8-9:00. Pins will be provided.
Presenter Guidelines	Even # posters = Session 1 Odd # posters = Session 2
Judging / Awards	Best Poster Award will be given out during closing on Sept 16
Contact	ctc.conference@ctc-germany.org

Poster numbers correspond to board locations – see the floor plan posted at registration.

POSTER #1

Nora Beier

Universität Leipzig, Germany

TBA

ABSTRACT

TBA

POSTER #2

Martin Rudolph

Leibniz Institute of Surface Engineering (IOM), Germany

Role of vibrationally excited states in oxygen plasma chemistry

ABSTRACT

Cold plasma discharges are an efficient tool for driving non-equilibrium chemistry: electrons can be heated to high energies while heavy species remain near room temperature. Such discharges give rise to an exceptionally rich variety of pathways for generating chemically active species. This applies in particular to molecular gases that, besides their electronic states, have a large number of closely spaced vibrational states. These states facilitate stepwise excitation processes, enabling access to highly excited, dissociated, or ionized states through interactions with electrons of comparatively low energy relative to the final state.

In this contribution, we employ a spatially-averaged (global) plasma chemistry model of oxygen to study the role of vibrationally excited states on the formation of atomic oxygen. The model self-consistently accounts for electron energy balance and species densities based on a detailed set of plasma-chemical reactions. Vibrational levels are populated by electron impact excitation from the ground state and lower-lying vibrational states, while detailed balancing is used for a consistent treatment of the reverse processes. Each vibrational state provides a distinct, reduced threshold for the production of atomic oxygen via electron-impact dissociation and dissociative electron attachment. The results show how the consideration of vibrational excitation in global models modifies atomic oxygen production pathways.

POSTER #3

Zhen-Hua Zhao

Nanyang Technological University - NTU Singapore, China

TBA

ABSTRACT

TBA

POSTER #4

Ma Tianjiao

Nanyang Technological University, Singapore

TBA

ABSTRACT

TBA

POSTER #5

Lin Congjian

Nanyang Technological University, Singapore

TBA

ABSTRACT

TBA

POSTER #6

Felix Moorhoff

Leibniz Institute of Plant Biochemistry, Germany

Co-Authors: Lilly Eger, David Medina-Ortiz, Mehdi D. Davari

SelectZyme: AI-Based Interactive Protein Space Visualization for Enzyme Discovery, Selection, and Mining

ABSTRACT

Enzymes are central to biotechnological innovation and play key roles in natural product biosynthesis, biocatalytic cascade design, and synthetic biology. Yet, the vast majority of enzymes encoded in genomic and metagenomic data remain uncharacterized, limiting our ability to exploit their catalytic potential for natural product discovery and industrial applications. Traditional enzyme mining approaches rely heavily on sequence similarity searches and alignment-based clustering, which struggle with sequence diversity and often require extensive manual curation and parameter optimization.

To overcome these limitations, we developed SelectZyme, an embedding-based enzyme mining and visualization platform that enables intuitive exploration of enzyme sequence spaces derived from protein language models. SelectZyme provides a user-friendly workflow that requires only a textual query to initiate analysis. The platform integrates unsupervised clustering and dimensionality reduction to generate interactive visualizations, including protein landscape plots, phylogenetic trees, and graph approaches such as minimal spanning trees. Researchers can select individual enzymes or entire regions of interest directly from the visualization and export annotated tables and plots for direct gene order for experimental validation.

By bridging advanced embedding models with accessible visualization, SelectZyme streamlines the discovery and prioritization of enzymes with potential roles in natural product biosynthesis and biocatalysis. The tool facilitates hypothesis generation and enzyme selection for researchers of all expertise levels, thereby accelerating the integration of computational enzyme mining into biosynthetic pathway elucidation and engineering.

POSTER #7

Dirk Heymel

Hochschule Merseburg, Germany

Co-Authors: Mathias Seitz, Stephan Schröter, Thomas Rothgänger

Catalytic Cracking of Polyolefins with Supported Catalysts in a Continuous Scale

ABSTRACT

In this work, the catalyst was immobilized on a carrier, which can subsequently be separated from solid residues for regeneration. However, a key challenge is to maintain high catalytic activity of the supported catalyst compared to the powder form. Pore size engineering is therefore essential to reduce limitations associated with pore diffusions. A second advantage of catalytic cracking is the possibility of achieving high gas yields with high fractions of ethylene, propylene, butenes, and aromatic compounds. Instead of cleaning and upgrading pyrolysis oil by hydrogenation followed by steam cracking to monomers, these gases can be readily purified using absorption techniques and directly fed into the downstream steam cracker. In contrast to classical pyrolysis, catalytic cracking predominantly yields low-molecular-weight compounds, which can be purified using absorption techniques. To implement this concept, the catalytic conversion of real plastic waste streams was investigated in a continuous reactor. The relationships between catalyst properties, waste feed quality, the process conditions and the resulting gas yield and composition were systematically examined. For this work, different types of polyolefinic plastic waste and different catalysts were used. As feedstocks, waste sorting residues from foil separation (M), which were defined as the standard case, as well as refuse-derived fuel (RDF) from municipal waste collection in Germany were employed. As catalysts, MFI zeolite powder immobilized on different carriers was used. The supports were commercial samples. Coating of the carriers was developed using specially designed binders with additives. The loading of the carrier material with MFI was approximately 10 wt%. The catalyst formulations were carried out at pilot scale and tested in different reactors. For continuous catalytic cracking, the aforementioned plastic waste was fed into a paddle reactor at temperatures between 430 and 600 °C. The catalyst-to-feed ratio ranged from 1:5 to 1:40. In a first step, the different catalysts were tested in a batch rotary kiln reactor. Two different supported catalysts and a reference, namely the original MFI in powder form. The first formulation differed in behaviour from the powder catalyst. Under screening conditions at 430 °C the product spectrum exhibited a higher wax content, while the desired olefin fraction (ethylene, propylene, and butenes) and other light fractions lower than from the powder catalyst. Using an alternative support with a similar catalyst loading, the product distribution was comparable to that of the powder form. This indicates that the second supported catalyst is capable of cracking polymers and waxes to a similar extent as the powder form. It exhibits nearly the same activity, and it appears that no significant macropore diffusion limitations occur. In the continuous reactor, the gas yield of catalyst 1 at 480 °C was 35% and that of catalyst 2 was 40%. Catalyst 2 delivered higher amounts of propene and butenes (gas yield 40%), while the proportions of pentenes and hexenes decreased. At temperatures of around 600

°C (gas yield > 90%), the thermal cracking dominates over catalytic cracking, but the catalytic influence remains, as pyrolysis without a catalyst leads to the undesirable formation of wax and coke. Catalytic cracking can lead to improved conversion of polyolefinic plastic waste streams into monomers such as ethene, propene, and butenes, which can be directly fed into the downstream section of a steam cracker. In contrast to conventional pyrolysis, catalytic cracking can avoid additional purification and conversion steps such as hydrogenation and steam cracking of pyrolysis oils. To achieve an optimum, the process conditions must be adapted for each waste stream. It can be shown that strong correlations exist between catalyst demand and waste quality, as well as the selected temperature. Modeling of these correlations is currently in progress.

POSTER #8

Bolun Wang

Institut für Technische und Makromolekulare Chemie, RWTH Aachen University, Germany

Co-Authors: Joel Britschgi, Ivana Jevtovikj, Piyush Ingale, Thomas Schaub, Stephan Andreas Schunk*, and Ferdi Schüth*

Recover polyol monomer from polyurethane via solvent-free mechanocatalytic hydrolysis with heterogeneous catalysts

ABSTRACT

Plastics with various functionalities are indispensable in modern society. Over 390 million tons (Mt) of plastics were produced worldwide in 2021. Around 21 Mt of the amount produced (5.5%) was polyurethane (PU), synthesized from a variety of polyols and isocyanates. PU is thus ranked as 6th in the list of the highest production volume plastics. While most of the collected plastic waste was mechanically recycled, the cross-linked structure of thermoset PU makes this physical recycling process not feasible.

The chemical recycling of plastics using small molecules (H₂O, H₂, O₂...) to break the polymeric network shows great potential to recover valuable feedstocks or even intact monomers for polymer production. The solvolysis of PU has been proven to be an efficient process to decompose PU into alcohol and amine, which can be reused for polymer production. Although the glycolysis of PU has been tested on a pilot scale, its market competitiveness is still limited by the reaction temperature (130-200 °C), the cost of excess glycol, and the reduced quality of products.

The solvent-free hydrolysis of PU via mechanochemistry could be a promising alternative pathway to recover polyol monomer from thermoset PU under milder conditions. In this work, we present our results (patent applied for) on the chemical recycling of commercial PU sponge via mechanocatalytic methanolysis and hydrolysis. Up to 80% soluble polyol can be recovered from the hydrolysis of toluene diisocyanate (TDI)-based PU, catalyzed by base and a Cu/MgO catalyst in a shaker mill with reagent amounts of H₂O.

The hydrolysis of PU is harder than its methanolysis, possibly due to the higher polarity of H₂O. The stronger adsorption of H₂O might saturate the active sites. Therefore, the yield of polyol significantly decreased when H₂O was added. It also can explain the 3-6 times lower yield of polyol produced in 20 mL MeOH or H₂O compared to this solvent-free mechanocatalytic process at the same temperature. Surprisingly, almost 80% polyol can be recovered from the hydrolysis of PU at 90 °C. In addition to the temperature effect, the Cu/MgO catalyst also plays an important role in the hydrolysis of PU. At 75 °C, the presence of Cu/MgO together with impregnated NaOH results in almost fourfold higher yields compared to the reaction only with NaOH. The impregnation of base is not necessary when Na₂CO₃ powder is employed, leading to moderate yields of polyol. As proof-of-concept, cross-linked PU has been successfully re-synthesized with the recovered polyol.

The solvent-free recycling process of PU allows a lower reaction temperature, only reagent amounts of liquid, and easier separation of products, which could make it more competitive than the conventional solvolysis pathways. This novel chemical recycling process for commercial PU products can successfully prevent unselective bond cleavage, which commonly happens during the hydrogenolysis of waste plastics.

POSTER #9

Doris Völker

German Environment Agency (UBA), Germany

Co-Authors: Kathrin Schwirn, German Environment Agency

The European Commission's Safe and Sustainable-by-Design Framework: Chances and Challenges to support the transition of the chemical industry

ABSTRACT

Safe and Sustainably by Design (SSbD) is a voluntary pre-market approach to guide innovators in the development of safe and sustainable chemicals, materials, processes, and products. It assists to identify and minimise the impacts concerning safety for humans and the environment, and for sustainability, taking a lifecycle perspective. By that, it helps innovators to steer to a green and sustainable transition by integrating safety and sustainability considerations into the (re-)design and development of products, processes, or technologies from the early stage of innovation.

At European level, SSbD was introduced as one of the key aspects of the EU's Chemical Strategy for Sustainability towards a toxic-free environment (2020) of the European Green Deal. In 2022, the European Commission published its first recommendation on establishing an European assessment framework for SSbD chemicals and materials. This recommendation was supported by a framework (developed by JRC) for the definition of criteria and an evaluation procedure on SSbD. In the following years this framework has been extensively tested and additional guidance for assessing SSbD has been given by a JRC methodological guidance. Based on the experience in applying SSbD, a new EC recommendation together with a revised EC assessment framework for SSbD chemicals and materials has been published in 2026.

The poster will present our perspective on the EC SSbD framework and highlight its strengths and remaining challenges to provide systematic information on safety and sustainability in early stages of development. It will also highlight the regulatory relevance of SSbD by showing the link between SSbD and EU legislation which include obligations with respect to safety and sustainability. By this, SSbD fosters early anticipation of regulatory obligations and facilitates regulatory compliance for later stages of innovation.

POSTER #10

Gabrielle Melo da Silva

Max Planck Institute of Colloids and Interfaces (MPIKG), Germany

Co-Authors: Miguel Garcia, Christian Hoffmann, Jens-Uwe Repke, Peter H. Seeberger, José Danglad-Flores

Evaluating Molecular Representations for Glycan Chemistry: From Descriptor to Prediction

ABSTRACT

Assigning glycosylation conditions remains challenging because practitioners lack systematic data-driven methodologies. As a first step toward future AI-assisted prediction of glycosylation variables such as concentration, time, and temperature, this study evaluated molecular descriptors as candidate molecular representations. PCA-based analysis showed changing descriptor contributions across sugar datasets, with increasing significance of 2D information as the number of aromatic protective groups increases. We predicted retention time as proof of concept to demonstrate a structure-property model. A compact set of descriptors can achieve strong performance while preserving chemical interpretability. Although learned representations yielded the highest overall accuracy, descriptor-based models remained highly competitive and provided clearer chemical meaning.

POSTER #11

Jonas Hoffmann

GreenDelta GmbH, Germany

Co-Authors: Max Bringmann, Ashrakat Hamed, Micheal Srocka

Using Retrosynthesis for Sustainability Assessment: An Automated Workflow for Life Cycle Sustainability Assessment of Safe and Sustainable by Design Chemicals

ABSTRACT

The planetary boundaries concept highlights that human activities are pushing Earth systems beyond safe operating limits, not only with regard to climate change, but also in areas such as acidification and freshwater change. In this context, novel entities, including synthetic chemicals, have emerged as a critical and growing concern. This underscores the need to ensure that newly developed chemicals are designed to be intrinsically safe and sustainable from the outset, rather than being assessed only after development or market entry. Within the European Safe and Sustainable by Design (SSbD) framework, as advanced by the Joint Research Centre (JRC), this requires integrating hazard, performance, and full life cycle sustainability considerations already at early stages of innovation.

At the same time, laboratories are increasingly adopting concepts such as Green Chemistry and Sustainable Chemistry, driving greater interest in methods for systematically evaluating sustainability. While Green Metrics and related process-level indicators are valuable for assessing synthesis efficiency, material use, and reaction-level greenness, they do not capture broader system-level trade-offs across supply chains, energy provision, use patterns, and end-of-life pathways. Hence, Life Cycle Sustainability Assessment (LCSA) provides a systematic framework for evaluating environmental, economic, and social impacts across the full life cycle of chemicals. However, its application remains challenging due to substantial data requirements and limited data availability, particularly in early development.

Herein we present an automated workflow that links retrosynthesis with LCSA to support the evaluation of chemicals in line with SSbD principles. Implemented in openLCA, the workflow starts from alternative synthesis pathways generated by digital retrosynthesis tools such as ASKCOS, IBM RXN, or AiZynthFinder. The workflow automatically translates their outputs into model-ready life cycle inventories, enabling systematic sustainability assessment of candidate synthesis routes. This allows not only to conduct environmental modeling which is complemented by economic assessment through LCC and by social hotspot analysis using databases such as PSILCA and SOCA, enabling a broader evaluation of sustainability trade-offs during chemical development.

While retrosynthetic approaches can mirror the production of chemicals, a particular focus is placed on end-of-life considerations. Rather than treating end-of-life as a fixed assumption, the proposed workflow predicts likely end-of-life pathways based on the composition and formulation of the

chemical and its expected application context. This is especially relevant for chemicals whose downstream fate, recyclability, emissions potential, or waste treatment routes vary substantially with formulation choices. By incorporating these prospective end-of-life scenarios, the workflow extends sustainability assessment beyond production and use-phase considerations and better reflects the full life cycle logic required by SSbD.

Overall, the proposed approach demonstrates how retrosynthesis can be used in an interdisciplinary fashion to automate life cycle inventory generation and sustainability assessment creating a practical decision-support tool for safer and more sustainable chemical innovation. It contributes to the operationalization of the SSbD framework by providing a transparent and scalable method for comparing alternative chemical pathways across environmental, social, and economic metrics.

POSTER #12

Ilayda Cayirlii

Leipzig University, Germany

Co-Authors: Arne Thomas, Matthias Drieß, Reinhard Schomäcker, Majd Al-Naji

Engineering Microviridin Macrocyclization as a Biocatalytic Tool

ABSTRACT

Microviridins are ribosomally synthesized and post-translationally modified peptides (RiPPs) containing characteristic lactam and lactone macrocycles installed by ATP-grasp ligases. Due to their high regioselectivity and mild reaction conditions, these enzymes represent promising biocatalytic tools for peptide engineering.

In this study, we combine computational and experimental approaches to investigate and engineer microviridin macrocyclases. AlphaFold and Rosetta are used to model enzyme–substrate interactions and evaluate the effects of targeted mutations on enzyme stability, substrate recognition, and catalytic activity. Based on computational predictions, selected mutants are generated and experimentally characterized.

Synthetic microviridin precursor peptides are used as substrates in enzymatic assays to evaluate how mutations influence macrocyclization efficiency and product formation. By integrating protein modeling, mutational analysis, peptide synthesis, and biochemical validation, this work aims to establish engineered microviridin macrocyclases as versatile platforms for selective peptide macrocyclization and biocatalytic applications.

POSTER #13

Muhammad Bilal

Technical University Berlin, Germany

Electrocatalytic Hydrogenation of Lignin Model Compounds on Supported Platinum Catalyst on Carbon

ABSTRACT

Lignin is the most abundant renewable aromatic source. Despite its potential, the complex polyaromatic structure of lignin poses a significant challenge for its depolymerization and valorization to drop-in chemicals. Lignin model compounds are investigated as they represent the key features of native lignin and are crucial to understand the catalytic performance and mechanistic pathways. Traditional upgrading methods include thermal catalytic hydrogenation (TCH) that requires harsh conditions resulting in undesired reactions, coke formation and catalyst deactivation. In this regard, electrocatalytic hydrogenation (ECH) emerges as a promising technique to valorize the lignin with controlled product selectivities, offering an alternative to conventional hydrotreatment processes. This approach is more advantageous than the conventional upgrading process, as it utilizes renewable energy for water splitting (in-situ hydrogen production), operates at mild conditions using aqueous solvent with no coke formation. Thus, this work is devoted to establish an understanding of e-cat hydrogenation of lignin monomers with different functionalities (such as 4-allyl phenol, eugenol, and 4-allyl syringol) using commercial 5 wt.-% Pt/C catalyst.

The ECH of eugenol and 4-allyl syringol was conducted in a homemade double-jacketed H-cell containing three electrodes (Pt/C coated on carbon cloth (working electrode), Ag/AgCl (reference Electrode), and Pt Spring (counter electrode) equipped with PEM. For each experiment, 10 mM of substrate was dissolved in 0.2 M HClO₄ with an applied current of -120 mA for 4 hours at 45°C. The obtained products were identified and quantified via GC-MS and FID.

The ECH was performed at different temperatures (RTP, 45°C and 65°C) to evaluate the catalytic performance of both substrates. Among these, 45°C was selected for discussion, as it provides balanced performance for conversion and product distributions. At 45°C, the ECH of eugenol results in full conversion with 4-propyl guaiacol as a major product while 4-propyl phenol, 4-propyl cyclohexanone, and 4-propyl cyclohexanol were the minor products. The overall faradaic efficiency (FE) was 19% after 1 h and it dropped after 4 h due to an increase in the hydrogen evolution reaction (HER). In contrast, 4-allyl syringol shows full conversion with only one selective product, i.e., 4-propyl syringol. After 1 h, the FE was 23%, but after 4 h, due to severe HER the FE was dropped to 7%. The high selectivity observed for 4-allyl syringol is attributed to the formation of a stable hydrogenated product that undergoes no further hydrogenation, whereas eugenol forms multiple products that compete for adsorption on the catalyst surface.

In summary, the nature of the substrate molecule greatly affects the catalytic performance, as eugenol showed multiple hydrogenation-deoxygenation pathways, while 4-allyl syringol showed chemoselectivity towards allyl hydrogenation.

POSTER #14

Tim Tegtmeier

Center for the Transformation of Chemistry (CTC)

Co-Authors: Tim Tegtmeier, Sascha Thinius, Laura König-Mattern¹

Towards Sustainable Surfactants: Conditional Surfactant Generation via Regression Transformer

ABSTRACT

Climate change and the depletion of fossil resources drive surfactant production from petroleum-based feedstocks towards environmentally friendly and renewable raw materials [1]. Desirably, next-generation bio-based surfactants (i) satisfy industrially relevant performance criteria, (ii) exhibit low toxicity towards aquatic organisms, and (iii) are economically viable to produce. To design such tailored surfactants, computer-aided molecular design frameworks enable the systematic exploration of the surfactant space. In this work, we introduce a Regression Transformer [2] that unifies property prediction and conditional molecule generation for the inverse design of surfactants within a single model architecture. The Regression Transformer [2], implemented with an XLNet backbone, uses permutation language modeling to obtain bidirectional attention while remaining autoregressive. Continuous properties are tokenized into digit tokens, resulting in numerical tokens (properties) that are jointly processed with textual tokens (molecular representations). Using transfer learning, we fine-tuned the Regression Transformer [2] pretrained on quantitative estimates of drug-likeness with surfactant-specific data, including critical micelle concentration (CMC), aquatic toxicity (LC_{50}), and synthetic accessibility (SA) score.

During fine-tuning, the Regression Transformer takes SELFIES molecular representations as inputs and learns to predict pCMC ($pCMC = -\log_{10}(CMC)$), aquatic toxicity, and SA score values that were normalized to [0,1]. Finally, we partitioned the dataset into training and validation set (80:20 ratio) using a stratified split, preserving surfactant types and aquatic toxicity distribution. The fine-tuned model, trained with early stopping based on validation performance, reaches $MAE_{val} = 0.471$ for pCMC, 0.644 for aquatic toxicity, and 0.252 for SA score. While existing models achieve similarly strong or slightly better predictive performance, they are typically limited to property prediction and lack generative capabilities. We apply the unified architecture to scaffold decoration tasks on lignin-derived molecular building blocks, such as phenolic monomers and oligomers obtained from biorefinery processes, with their most reactive positions masked. The transformer fills these positions conditioned on target ranges for CMC, aquatic toxicity, and SA score. Leveraging this unified architecture, the model enables the conditional generation of novel lignocellulose-based surfactants aligned with circular bioeconomy principles.

References: (1) R. Marquez, M. S. Ortiz, N. Barrios, R. E. Vera, A. J. Patino-Agudelo, K. A. Vivas, M. Salas, F. Zambrano and E. Theiner, *J. Surfactants Deterg.*, 2025, 28, 25–76.

(2) J. Born and M. Manica, *Nat Mach Intell*, 2023, 5, 432–444.

POSTER #15

Uwe Scheithauer

TU Dresden, Germany

Co-Authors: Hannah Knobloch, Stefan Holtzhausen, Hajo Wiemer

Additively Manufactured High-Performance Ceramic Components for Advanced Chemical Process Engineering

ABSTRACT

Chemical process engineering is often constrained by conventional manufacturing methods and materials that limit geometric complexity, functional integration, and operational performance. Consequently, highly efficient heat and mass transfer structures, corrosion-resistant process equipment or miniaturized devices are difficult to realize using established approaches. These limitations hinder progress in energy efficiency and operation under harsh chemical conditions.

To address these challenges, additively manufactured high-performance ceramic components are developed. Ceramic additive manufacturing enables the fabrication of application-specific and geometrically complex structures, including static mixers, heat exchangers, reactors, or fluidic nozzles. Different ceramic materials provide exceptional thermal stability, corrosion resistance and mechanical durability, making them highly suitable for demanding process environments. Their high temperature resistance furthermore enables regeneration and cleaning by pyrolysis at temperatures of 1200°C and higher.

By combining advanced ceramic materials with additive manufacturing, functional properties can be fully exploited in optimized component designs that improve heat and mass transfer while reducing system size and material consumption. Components can be miniaturized, tailored to specific process requirements, or include the integration of additional features. Furthermore, selected additive manufacturing approaches enable the integration of multiple ceramic materials within a single manufacturing step. This, for example, allows the combination of porous and non-porous regions, or electrically conductive and insulating ceramics, within one component. As a result, functionalities such as integrated heating elements or temperature sensors can be directly incorporated into process equipment.

In addition, computational design and process-specific optimization are leveraged to develop next-generation ceramic process components with improved thermal management, better energy efficiency, or increased system compactness.

A representative example is the development of additively manufactured ceramic static mixers with application-specific geometries tailored to different fluid systems and process conditions. Through computationally optimized design, mixing efficiency can be significantly enhanced while simultaneously reducing pressure loss. In addition, the use of ceramic materials improves component lifetime (factor 10 and higher) due to their high resistance to mechanical abrasion and

chemically aggressive media. Strategically placed, spatially resolved temperature sensors inside the mixers enable a level of process monitoring previously unattainable, while integrated heaters allow for customized heat generation.

The presented approach demonstrates how digital design and additive manufacturing of ceramic materials can contribute to more efficient, robust, and sustainable chemical processing technologies. At the same time, this enables continuous in-situ process monitoring and control and establishes the data foundation needed to use AI to better understand and optimize the processes taking place inside.

POSTER #16

André Busching

Leipzig University, Germany

Co-Authors: Berthold Kersting

Coordination Chemistry and Extraction Studies of Rare-earth elements - Past, Present and Future Studies utilizing Calix[4]arenes

ABSTRACT

Calixarenes represent a prominent class of macrocyclic host molecules in supramolecular coordination chemistry, distinguished by their structural preorganization and versatile functionalization, which enable highly selective binding of metal ions and molecular guests through non-covalent interactions and coordination bonds. Owing to these features, calixarene derivatives have found broad application in areas such as molecular recognition, catalysis, and environmental remediation.

Rare-earth elements (REE) are critical metals essential for a wide range of technologies pivotal to the clean energy transition, including the production of permanent magnets, luminescent materials, ceramic supports for exhaust emission catalysts, and catalysts for petroleum cracking and steel deoxygenation. With the rising demand for REEs and to mitigate potential supply shortages, caused by trade conflicts, the development of suitable recycling technologies is imperative.

In this contribution, we highlight past, present and future endeavours in the area of calix[4]arene-based agents for rare earth element extraction and separation performed by the Kersting group. Focussing on a comprehensive characterization of our complexes, elucidating the specific metal coordination environment by means of single-crystal X-ray diffraction (SC-XRD), complemented by spectroscopic techniques and quantum chemical calculations. This combined experimental and theoretical approach provides insight into the structure–property relationships governing metal coordination by the calix[4]arene framework and allows for the evaluation of potential real-world application of such systems.

POSTER #17

Marlen Zschätzsch

Technical University of Dresden, Germany

Co-Authors: Tristan Beihnsner, Katrin Hayn, Anett Werner

Bioabbaubare Mycel-basierte Komposite: Materialien für ein recyclingfähiges Autos

ABSTRACT

The excessive use of fossil-based plastics and the lack of a functioning circular economy are leading to severe environmental and health issues, such as microplastic accumulation in ecosystems and food chains. To address this, fully recyclable and biodegradable alternatives are urgently needed. While materials like lignin-based composites only cover a limited range of plastic properties, mycelium-based composites (MBC) offer a promising solution. These composites consist of a matrix of lignocellulosic substrates, such as wood granules or fibers, bound together by mycelium - a dense, filamentous network of fungal hyphae - offering a bio-based alternative for lightweight, porous materials.

We propose using MBC for automotive interior door panels, building on our prior research that developed lightweight insulation materials with a density of $\sim 100 \text{ kg/m}^3$. Using *Ganoderma lucidum* and miscanthus as a substrate, panels up to $110 \times 72.5 \times 12 \text{ cm}$ were produced, showing normal flammability (B3), high porosity (0.9), and low thermal conductivity ($0.044 \text{ W/(m}\cdot\text{K)}$). These properties make MBC a sustainable, functional alternative to plastics in automotive applications.

By utilizing mycelium composites as a base material for automotive applications, we can move closer to achieving a 100% sustainable and circular material economy. Not only do these materials address environmental concerns, but they also showcase the feasibility of replacing fossil-based plastics with renewable and biodegradable alternatives in industrial applications. We would like to present our vision and research findings on mycelium-based composites (MBC), with a focus on their application in vehicle interior design highlighting the transformative potential of mycelium-based materials and their role in shaping a more sustainable future for the automotive industry.

POSTER #18

Samuel Vitor Saraiva

Center for the Transformation of Chemistry, Germany

Co-Authors: Pranali Wankhede, Jose A. Danglad-Flores, and Peter H. Seeberger

TBA

ABSTRACT

Automation streamlines high-throughput chemistry, yet many solutions remain costly and complex. Digital twins, common in industry, are seldom used in research labs. This work introduces software that creates digital twins while automating hardware control. It features graphical design abstraction, asynchronous protocol processing, API-driven hardware communication, and interactive simulation management, offering a user-friendly, integrated approach to building and managing autonomous chemistry platforms.

POSTER #19

Paul Schebek

University Leipzig, Germany

Computational Design of Vanadium-dependent haloperoxidases for green chemistry

ABSTRACT

Halogenation reactions are among the most widely used transformations in synthetic organic chemistry. However, traditional methods frequently require toxic and environmentally impactful reagents. Vanadium-dependent haloperoxidases (VHPOs) offer a sustainable alternative, enabling less harsh reaction conditions by utilizing only benign halide ions and hydrogen peroxide as reagents.

Our goal is to provide sustainable biocatalytic options by developing engineered VHPOs for diverse biosynthetic applications, ultimately replacing traditional halogenation chemistry. To achieve this, we are optimizing the stabilization and recombinant expression of known VHPOs to enhance their thermal stability, catalytic activity, and substrate scope. This approach couples computational design workflows with rigorous experimental validation.

Additionally, we are developing entirely new, de novo protein scaffolds that harbor the native catalytic reactivity of VHPOs. This allows us to generate hyper-stable, custom-tailored enzymes with bespoke substrate-binding sites designed for targeted applications in organic synthesis. Together, these strategies establish a robust framework for expanding the utility of eco-friendly halogenation in chemical manufacturing.

POSTER #20

Jan Rossa

Institut für Wirkstoffentwicklung, Universität Leipzig, Germany

Co-Authors: Stefan Arnhold, Jens Meiler

Chemistry competition to identify, support and challenge talents

ABSTRACT

„Chemie – die stimmt!“ (CDS) is a four-stage student competition for grades 8 through 10, organized by "Förderverein Chemie-Olympiade" and administered by the Institute for Drug Discovery at the University of Leipzig. Founded in Leipzig in 2000 to serve the central German states Saxony, Saxony-Anhalt and Thuringia, the competition has undergone continuous expansion and was officially recognized as a national competition by the Conference of Ministers of Education and Cultural Affairs in 2021. As the largest nationwide chemistry competition, CDS serves as the link between existing regional experimental competitions and the selection process for the International Chemistry Olympiad. Spanning the journey from the first competition stage—which recently attracted 5,100 participants—to the national final in Leipzig featuring the top 36 contestants, CDS transitions from broad-based engagement to the targeted promotion of elite talent. Our objective is to inspire students to pursue chemistry—specifically during the grade levels when all career paths remain open—and to identify, nurture, challenge, and network those who demonstrate exceptional talent. Over the past 11 years, 81% of the finalists in the selection process for the International Chemistry Olympiad—representing Germany's top 15 young chemists—were former CDS participants. As a next step in our expansion, we are planning a support program specifically for German schools abroad. These schools educate 85,000 German-speaking students and have the potential to contribute significantly to alleviating the shortage of skilled professionals in the STEM fields.

POSTER #21

Lunhan Chen

BasCat - UniCat BASF Joint Lab, Germany

Co-Authors: Cassian Herr, Raoul Naumann d'Alnoncourt, Michael Geske, Michael Bender, Frank Rosowski, Majd Al-Naji

Hydrocracking of Polyethylene: The Effect of Catalyst Support and Reaction Conditions on the Product Distribution

ABSTRACT

Only a small fraction of approximately 12% of plastic waste world-wide undergoes mechanical recycling, which is limited to pure polymer waste streams. Therefore, the development of chemical recycling to increase the amount of recycled plastic materials is crucial. Among available recycling techniques, catalytic hydrocracking has the advantage of the production of valuable saturated hydrocarbons from a mixture of plastics within a single step.

The conventional hydrocracking mechanism was reported on a bifunctional catalyst, featuring acid sites cracking intermediates down to shorter fragments and metal sites hydrogenating C-C bonds. The distinct roles of each catalyst component need to be understood better, in order to tune the relevant properties to optimize catalyst performance. Additionally, the influence of reaction conditions such as the effect of hydrogen depletion at lower hydrogen pressures or hydrocracking throughout ongoing reaction time are often lacking a detailed product spectrum analysis.

In this work, the hydrocracking of Linear Low Density Polyethylene (LLD-PE) is studied on model catalysts with 1wt% Pt loaded on Zeolite Beta (HCZB150, Si/Al = 150, Clariant) and amorphous silica-alumina with high pore volume (ASA70 HPV, 70% SiO₂, Sasol). The hydrocracking experiments were performed in a stainless steel autoclave (300 mL) with 50 g LLD-PE and 10wt% catalyst loading. Reaction conditions are tested to investigate the effect of H₂ pressures (20 – 60 bar at room temperature) and reaction times (0 – 12h). The H₂ conversion and product distribution (C₁-C₅, gas) were quantified with GC-FID/TCD, while C₆-C₂₂ products (liquid) were identified and quantified with GC-MS/-FID. Higher molecular products (C₂₂+) are analyzed with simulated distillation and GPC.

Hydrocracking of LLDPE with Pt/HCZB150 results in a faster conversion to mainly gas and liquid products already after 3 h, which could be attributed to the higher number of Bronstedt acid sites (52 $\mu\text{mol/g}$, Py-FTIR) compared to ASA70 HPV (22 $\mu\text{mol/g}$, Py-FTIR), on which the C-C cracking of polymer chains occurs. The product distribution consists of mainly low boiling alkanes below C₉, likely due to size exclusion effects of the micropores, which aligns with the reported templating role of the supports porosity. In contrast, the mesoporous catalyst Pt@ASA70HPV cracks LLDPE first into macromolecular products (C₂₂+), before reaching a high liquid yield with a broader product distribution with its maximum between C₆ – C₁₂. This catalyst system was also tested at a lower H₂ pressures, which resulted in the formation of aromatic compounds, due to hydrogen depletion.

The results highlight the importance of the choice of support in the catalyst system as well as the hydrocracking reaction conditions in order to obtain the desired product distribution.

POSTER #22

Christoph Herfurth

Fraunhofer Institute for Applied Polymer Research IAP, Germany

Co-Authors: Daniel Zehm, Antje Lieske

Synthesizing Circular Carbon Polymers: Polyesters, Polyamides, and Polyurethanes

ABSTRACT

Fossil carbon sources are becoming increasingly unfavorable due to problems with access and availability as well as adverse effects on the environment. Hence, alternative carbon sources get more and more attention. Various approaches are being developed, from using bio-based carbon or CO₂ to chemical recycling of polymers. All these concepts share a certain level of circularity to minimize the amount of new fossil carbon needed for industrial processes.

This contribution investigates multiple ways of synthesizing polymers for circular carbon use, and the optimization of their material properties to make them fit for application. Starting from the synthesis of bio-based polyesters like PBS and PLA, as well as polyamides. Here, insights into the relation between material, process and properties are given. The second section focuses on chemical recycling on both polyesters and polyamides, presenting challenges and solutions for the use of monomers from different sources.

The main focus will be on the development of CO₂-based non-isocyanate polyurethanes (NIPUs) and their application for tubing, foams, and adhesives. Here, a new way to CO₂-based dicarbamates is shown, as well as their use as building blocks for NIPUs.

POSTER #23

Frank Lange

Leibniz Institute of Plant Biochemistry, Germany

Co-Authors: Fabian Mauz, Frank Broda, Ludger A. Wessjohann

The ABCDEE Extractor: automating the extraction of structured information on natural products from the scientific literature

ABSTRACT

Comprehensive collections of information on natural products (NPs) underpin the discovery and development of novel therapeutics. However, manual curation of NP databases is labor-intensive and cannot scale with the ever-growing publication output on NP isolation and characterization, which makes automation of extraction and curation processes indispensable.

To address this bottleneck, we present our ideas and first implementations of an information extraction pipeline from unstructured text documents such as scientific articles, which is developed within our ABCDEE project (Automated Bio-Chemical Data Extractor & Explorer). The pipeline consists of different machine-learning (ML) and database-based modules, for instance optical chemical structure recognition (OCSR), name and synonym lookups and classifications of chemical compounds and natural language processing via the invocation of large language models (LLMs). We specifically aim to use small and open-weight models that can be deployed on in-house hardware. Our strategy is to supply as much useful information as possible to the LLM in the initial prompt and "interactively" during LLM processing using function/tool calls without human intervention. Parsing of the LLM's natural language response can be avoided by enforcing structured data generation with an arbitrary output scheme, thus achieving uncomplicated downstream processing and integration as a dataset.

POSTER #24

Francesco Brandi

National Research Council, Institute of Chemistry of Organometallic Compounds CNR-ICCOM, Italy

Co-Authors: Carmen Moreno-Marrodán, Francesca Liguori, Pierluigi Barbaro

Depolymerization of polyesters polyol polyurethane using heterogeneous catalysts

ABSTRACT

Polyurethanes (PU) account for 5 wt% of global plastic market, corresponding to 28 Mt y⁻¹ of production. Generally, PU are a complex and wide class of polymers with a composition and formulation tailored for the specific application. Therefore, PU recycling is still extremely challenging. Among PU components, polyester polyols represent 10% of the polyols, generally used for flexible foams.

Catalytic chemical hydrogenolysis of PU is a promising approach in which PU are depolymerized with the action of a redox catalyst. Up to date, there are few examples of such an approach in literature, mostly focusing on homogeneous catalyst (Ru, Mn, and Ir-pincer) with the addition of mineral bases.

In this work, we investigated the combined alcoholysis and hydrogenolysis of a toluene diisocyanate(TDI)-polyester commercial-grade polyurethane foam using EtOH as a green solvent and solvolysis agent with Ru/Al₂O₃ as heterogeneous catalyst and in absence of any mineral bases. The process enables selective depolymerisation of cross-linked PU networks into monomers, including linear carboxylic diethyl esters, glycols, and N-alkylated aromatic diamines, achieving up to 85 wt% cumulative monomer yield (225 °C, 10 bar H₂, 17 h). The study highlights the role of Ru/Al₂O₃ in presence of H₂ to promote synergistic solvolysis–hydrogenolysis pathways, offering a promising circular alternative to landfill disposal and advancing catalytic strategies for PU upcycling.

The selected Ru/Al₂O₃ catalyst was used to depolymerize the TDI-polyester commercial foam. The conversion was found to be quantitative, with the alkyl diesters (diethyl-glutarate, -adipate, and -succinate) as the major products. In addition to the diester, alkylated diamines emerged as secondary byproducts. Overall, the cumulative monomer yield was of 51 wt.% of initial PU sponge. Additionally, optimisation of reaction parameters, such as pressure, temperature and time, resulted in an optimum cumulative yield of 85 wt% at 225°C.

In conclusion, this study demonstrated that heterogeneously-catalysed PU hydrogenolysis/alcoholysis is a promising approach toward a plastic circular economy.

POSTER #25

Aleksandra Olshanova

Department of Mathematics and Computer Science, University of Southern Denmark, Odense, Denmark; Faculty of Mathematics and Computer Science, Friedrich Schiller University Jena, Jena, Germany.

Co-Authors: Jakob Lykke Andersen, Rolf Fagerberg, Daniel Merkle, Christoph Flamm, Peter Dittrich

Molecular design using learnable graph grammars

ABSTRACT

De novo molecular design is the automated process of proposing novel chemical structures that aim to satisfy a desired molecular profile. In recent years, many computational approaches have been developed relying on deep neural networks. Although deep generative modeling techniques have significantly improved the generation and optimization of molecules, they often require large datasets and produce less interpretable models. In addition, they sometimes generate molecules that are difficult or impossible to synthesize. Most of these models have so far been developed specifically for SMILES sequence generation, but the ambiguity of SMILES has motivated a shift toward graph-based molecular representations. For instance, some methods work directly with the molecular graph and construct molecules according to elementary operations that maintain chemical valence rules.

In this work, we propose a framework for de novo molecular design that extends recent methods. Our methodology represents molecules as graphs and uses a learnable graph grammar to construct chemically valid structures. Starting from a domain-specific compound dataset, we identify recurrent structural motifs by iteratively applying frequent subgraph mining techniques. These motifs are then converted into graph transformation rules that maintain their connectivity within the molecule and to each other. After removing the most common motifs, we repeat the process until all parts of the initial molecules have been removed.

The resulting graph grammar can now guide the construction of new candidate molecules by iteratively applying rules in a probabilistic manner. Generated molecules are evaluated based on target properties, and the feedback is used to update the grammar. Specifically, the grammar learns conditional probabilities: the likelihood of applying a rule given the sequence of previous rules. This way, the generation process becomes adaptive, favoring rule sequences that produce molecules closer to the desired properties.

The developed method ensures the generation of novel, property-optimized, chemically valid molecules using interpretable and rule-based learning framework.

POSTER #26

Juliane Schmidt

PTS - Institut für Fasern & Papier gGmbH, Germany

Co-Authors: A. Feldner, G. Schaper, M. Röllig

Wheat Straw as a Renewable Fiber Source: Thermochemical Extrusion for Sustainable Pulp Production

ABSTRACT

Waste paper is an important resource for the paper industry and integral part in the sustainability of paper products. However, the quality of recycled fibres decreases continuously over the recycling cycle, as fibres progressively lose length and structural integrity due to repeated processing, mechanical stress, and chemical degradation. In addition, the availability of high-quality primary fibres within the recycling stream has also been declining for years. The decline of graphic paper since around 2005, driven by the ongoing digitalization of media and office communication, has led to significantly reduced inputs of high-quality primary fibres into the waste paper stream, thereby increasingly limiting the raw material base for certain paper and packaging applications. To counteract this decline in fibre quality, paper producers look for alternative fibre feedstocks to supplement recycled fibres in paper production. Considering that approximately 8–13 million tonnes of wheat straw are sustainably utilizable each year in Germany, wheat straw represents a promising alternative lignocellulosic fibre source. In this study, we investigate the suitability of wheat straw as an agricultural residue for the production of unbleached high-yield pulp.

In a novel pulping process, wheat straw was processed in a co-rotating twin-screw extruder under high-consistency conditions in an alkaline medium, combining mechanical, thermal, and chemical treatments to obtain a material resembling chemo-mechanical pulp, suitable for paper production. In a subsequent step, the resulting pulp was separated from the pulping liquor containing the extracted lignin. In several systematic experimental stages, the influence of key process parameters – particularly equivalence ratio, NaOH concentration, screw speed, and process temperature – on fibre morphology and energy consumption was investigated. After optimization of the extrusion and washing process, laboratory paper sheets were prepared from the obtained straw pulp and evaluated with respect to their mechanical and barrier properties.

Overall, the study demonstrates that twin-screw extrusion shows strong potential for the sustainable utilization of agricultural residues and represents a promising contribution to circular paper production.

POSTER #27

Janine Hauer

Luther University Halle-Wittenberg, Germany

Co-Authors: Network "Social Studies of Chemicals and Chemistry in Transformation" (S2C2): Patrick Bieler (Technische Universität München), Ruzana Liburkina (Universität Hamburg), Thomas Roiss (Technische Universität München), Christian Schnurr (Technische Universität München), Nona Schulte-Römer (Technische Universität Dresden)

Shaping Chemosocial Worlds: A Collaborative Proposal

ABSTRACT

The transformation of the chemical industry is on everyone's lips. While the goal of establishing a circular economy based on renewable energy and raw materials for a sustainable future is widely shared, the conditions under which this transformation takes place prove to be highly context-specific: political programs, legal frameworks, historical trajectories, economic dependencies and obligations, as well as social and cultural patterns vary to different degrees between sites. Every transformative effort therefore has to navigate between these local dimensions and global objectives.

We argue that qualitative science and technology studies (STS), as we propose them here, offer an opportunity within this complex constellation to make actual and potential path dependencies visible and open discussions through the research-based accompaniment of everyday practices of navigation and decision-making as they emerge. At the same time, such research provides valuable insights into the modes of thinking and working within chemical research and industry. These insights can form the basis for nuanced translations of "chemo-industrial concerns" to broader publics, thereby fostering "chemical literacy" and encouraging broader societal engagement with chemical processes and transformations.

We propose the joint development of formats and forums that complement the downstream and evaluative role often assigned to social-scientific technology research. Instead, we advocate establishing a simultaneous, exchange- and discussion-oriented collaboration as an integral component of transformation processes themselves.

POSTER #28

Camila Dias

BasCat – UniCat BASF JointLab, Technische Universität Berlin, Germany

Co-Authors: Sophie Peries, Philipp Wegener, Michael Geske, Markus Antonietti, Peter Neubauer, Majd Al-Naji and Frank Rosowski

An Integrated Approach from Wood Fractionation to Hydrodeoxygenation for the Formation of α,ω -Diol

ABSTRACT

Hemicellulose is an underutilized fraction of wood, composed by C5- and C6-sugars. Pretreatment processes like reductive catalytic fractionation often leads to its degradation, causing loss of 20 – 30 wt.% of the biomass. Therefore, there is a need for the development of methods like hydrothermal fractionation, where this fraction is utilized. However, after fractionation products are obtained, challenges are present in the conversion of these compounds into chemicals of interest, e.g., α,ω -diols.

The development of efficient and selective catalysts for hydrodeoxygenation reactions are a challenge in the study of biorefineries. Especially in the production of α,ω -diols, like 1,6-hexanediol (1,6-HDO). In the conversion of 1,2,6-hexanetriol (1,2,6-HTO) into 1,6-HDO, bimetallic catalysts stand out as an option that presents high selectivity. The best example being Pt – WO_x supported on titania, where the high selectivity observed is credited to the synergistic effect between Pt and WO_x and the reducible support. The current study looks into these challenges and presents initial testing to better understand this catalyst behavior under varying conditions.

The 4 wt.% Pt – 4 wt.% WO_x catalyst supported in titania was prepared through a 3-step incipient wetness impregnation. The catalytic testing was performed in an in-house constructed trickle-bed reactor. The catalyst was tested from 150 °C to 250 °C, increasing 25 °C in each measurement.

The conversion of 1,2,6-HTO and the selectivity towards 1,6-HDO varies greatly with the temperature. With its increase, a clear "over hydrodeoxygenation" can be observed, with an increase in selectivity towards monoalcohols. At the same temperatures, the formation of more C5 compounds can be observed, indicating bond cleavage involving a terminal carbon. This reaction is highlighted by the production of 1,5-pentanediol (1,5-PDO) and 1,2-pentanediol (1,2-PDO). While there is a significant increase in conversion, a decrease in 1,6-HDO selectivity is observed. Due to these variations, the highest yield observed is of 33% at 225 °C.

The effects of the support, Pt mass loading, and the presence of WO_x on the reaction network are analyzed.

POSTER #29

Michael Goepel

Institute of Chemical Technology, Universität Leipzig, Germany

Co-Authors: Florian Maximilian Harth, Miha Grilc, Roger Gläser

Conversion of alga-derived glycolic acid in the aqueous phase using supported ruthenium catalysts

ABSTRACT

The concept of using microalgae as photobioreactors converting carbon dioxide and sunlight into metabolism-based platform chemicals, which are excreted into a surrounding medium for direct further conversion (also coined "New Green Chemistry") is very promising. It poses several advantages over the conventional concept of growing, harvesting and processing biomass before further chemical upgrading. However, also challenges derive concerning catalyst activity and stability in the presence of the nutrient medium necessary for the microalgae-based production of platform chemicals. In this study the conversion of glycolic acid (GA) produced photobiocatalytically (via the new green chemistry approach) to ethylene glycol (EG) is studied.

The influence of support properties on catalytic activity for several supported metal catalysts in the conversion of a model aqueous GA-solution was investigated and ruthenium (Ru) was found to be the most promising active phase. Further the reducibility (influenced by catalyst-support interactions) of the active Ru species (in combination with Ru dispersion) is identified as key criterion for high catalytic activity. Textural and acidic properties are found to have no major impact on catalytic activity.

In a second study the effects of the necessary additives to the nutrient solution for microalgae-based GA-production on the catalytic activity of a commercial Ru supported on activated carbon catalyst (Ru/C) are systematically investigated. Sulphur and nitrogen containing metabolic inhibitor molecules in the nutrient solution and the type of acid used for pH-adjustment are identified as most important influences on catalytic activity in the conversion of GA to EG. The nutrient salts added and buffers used in the biotechnological medium were found to be less impactful. With this knowledge the photobiotechnological process of GA production was optimized and the subsequent conversion of an authentic alga-derived solution yielded 21 % EG under unoptimized conditions using a commercially available Ru/C catalyst.

In a third approach the use of bimetallic catalysts to reduce the amount of noble metal needed for GA conversion and increase catalytic activity is investigated. For this, the effect of adding platinum, palladium and rhenium to ruthenium creating supported bimetallic catalysts was investigated. The combination of ruthenium with rhenium is identified to be most promising. Both the metal ratio (optimum at $(n_{\text{Re}}) / (n_{\text{Ru}}) = 0.6$) and the impregnation sequence strongly influence the catalytic behavior of the bimetallic catalysts. In particular, impregnation of Ru onto a monometallic Re/AC

catalyst was beneficial due to significantly enhanced Ru dispersion, which results in ca. 25 % higher metal content-related conversion of GA.

Lastly microkinetic modeling of the reaction network of GA conversion to EG in the aqueous phase using a Ru/C at 120-180 °C was conducted. By considering possible (unwanted) reaction pathways (mainly acetic acid (AcA) formation) and multiple possible reaction intermediates a catalytic reaction pathway network and a kinetic model was proposed. The highest selectivity (70%) to EG was observed at 120 °C. At temperatures above 150 °C EG yield decreases despite higher GA conversion due to AcA formation. The modeling results can be the basis for a further experimental optimization of real algae-derived GA solutions.

POSTER #30

Bonnie Winter

Martin Luther University Halle-Wittenberg, Germany

Co-Authors: Raika Milde, Mahdi B. Helabad, Franziska Seifert, Markus Pietzsch, Martin J. Weissenborn

Enzymatic Detoxification of Deoxynivalenol by Thermostable Glutathione S-Transferases and Computationally Guided Protein Engineering

ABSTRACT

Deoxynivalenol (DON) is one of the most prevalent mycotoxins in Europe and is produced by *Fusarium* fungi infecting crops. DON contamination above regulatory limits of 5 ppm prevents the use of affected biomass as food or feed, causing substantial economic losses and food waste. Conventional physical and chemical detoxification strategies are often insufficient, non-specific, or incompatible with preserving feed quality. Enzymatic detoxification therefore represents a selective and sustainable alternative.

Glutathione S-transferases (GSTs) are particularly promising for DON detoxification, as they catalyze glutathione-mediated opening of the epoxide ring, a key structural motif contributing to DON toxicity. In addition, GSTs are attractive biocatalysts because they are independent of complex cofactors and rely solely on the co-substrate glutathione (GSH), which is naturally present in millimolar concentrations in plant cells. DON-converting GST activity has previously been reported for Fhb7 and the less characterized TrGST-C02, however, limited thermostability of Fhb7 ($T_m = 37.4$ °C) restricts practical application.

In this work, we identified and characterized GST homologs that retain DON-converting activity while exhibiting improved thermostability. Four of five fungal Fhb7 homologs and two of five plant-derived TrGST-C02 homologs were successfully expressed. All expressed homologs showed increased unfolding onset temperatures and melting temperatures (except of ThGST) compared to Fhb7. Among the fungal GSTs, PgGST displayed the highest thermostability, with a T_m of 48.4 °C, 11 °C higher than that of Fhb7.

While the plant-derived GSTs showed no detectable DON activity, all four fungal homologs converted DON, with PgGST reaching approximately 80 % of the activity of Fhb7. PgGST was therefore selected as a thermostable, catalytically competent scaffold for ongoing computational enzyme engineering. We are currently evaluating a FuncLib-based design strategy combined with automated docking, geometric filtering, and MM/PBSA-based binding energy estimation to prioritize designs for reduced apparent K_m and improved DON conversion.

This work contributes to sustainable and circular strategies for valorizing DON-contaminated agricultural streams by combining enzymatic detoxification with computational protein engineering.

POSTER #31

Clara Scheelje

TIB – Leibniz Information Centre for Science and Technology, Hanover, Germany

Co-Authors: Inka Marten, KIT-Library, Karlsruhe Institute of Technology; Nicole Jung, Institute of Biological and Chemical Systems (IBCS), Karlsruhe Institute of Technology

ChemPortal – Connecting Scientific Knowledge in Chemistry

ABSTRACT

Chemical research generates vast amounts of data daily, from synthesis protocols and spectroscopic analyses to quantum chemical calculations. However, this information is frequently fragmented across disparate sources, such as proprietary databases, non-searchable PDF documents, lab notebooks, and traditional journal articles. Further, chemical knowledge is often not machine-readable, hindering automated analyses, AI-driven discoveries, and efficient knowledge integration.

The DFG-funded Specialised Information Service for Chemistry (Fachinformationsdienst für die Chemie – FID Chemie), which started in February 2026, will address these challenges by offering the open web-based platform ChemPortal that summarizes, combines and promotes services that foster the gain of chemistry information. While integration into the library community ensures the systematic curation of information sources and provides comprehensive chemistry-related collections, innovative approaches to presenting scientific knowledge are simultaneously being developed.

The talk gives an overview about the most relevant aspects of ChemPortal and introduces one of ChemPortal's projects, the Open Chemistry Knowledge Base. This platform aims at the community-driven collection of information, designed to make chemical knowledge machine-readable, semantically linked, and openly accessible. Operating on Semantic MediaWiki, the platform allows researchers to directly input, link, and annotate molecular structures, properties, and experimental data. Unlike classical publication systems that produce static documents, this environment consists of dynamic, standardized, searchable, and machine-processable knowledge units. It thus offers an alternative to the traditional publication model: information is immediately available under an open access model, can be used to build dedicated databases based on chemical information, and can be curated by the community.

The ChemPortal project is carried out jointly by the Library and the Institute for Biological and Chemical Systems (IBCS) of the Karlsruhe Institute of Technology (KIT), as well as the TIB Leibniz Information Centre for Science and Technology. Our partners and supporting institutions include, amongst others, chemical societies, research institutions, libraries, and related NFDI consortia. The contribution will outline the vision of the project and demonstrate the synergy between community input and library oversight.

POSTER #32

Carla Terboven

Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Germany

Co-Authors: Michelle Browne, Matthew Mayer, Marcel Risch, Tobias Sontheimer, Michael Götte

Standardization as the Bridge: Integrating Manual and Automated Electrochemical Workflows with NOMAD and voc4cat

ABSTRACT

Modern electrochemistry depends on an ecosystem that combines automated and manual laboratory processes with both human expertise and emerging AI-agent decision-making. Realizing this ecosystem requires more than new instrumentation: it demands standardized, machine-readable descriptions of experiments and data so that results from heterogeneous sources can be compared, reused, and acted upon.

At Helmholtz-Zentrum Berlin (HZB), we develop digital workflows for electrochemical energy-conversion processes, including the hydrogen evolution reaction (HER), the oxygen evolution reaction (OER), and electrochemical CO/CO₂ conversion across multiple research groups. Our approach builds on the open-source research data platform NOMAD together with the catalysis vocabulary voc4cat, maintained by the NFDI4Cat consortium, to provide a common framework for integrating manual and automated laboratory workflows. Rather than treating manual experimentation as a problem to be eliminated, we deliberately preserve its flexibility and use it to identify the specific steps where automation delivers the greatest benefit.

In this contribution we present the digital workflows developed across our groups, focusing on the data schemas we have built for electrochemical measurements in NOMAD and on the integration of data analysis directly into these workflows to support scientists at the bench. We discuss how this combination of standardized schemas and embedded analysis provides a credible foundation for autonomous laboratories. Finally, we introduce the recently launched ASCEND project, through which we are automating laboratory processes to create a rich environment that joins manually and automatically generated data, yielding FAIR datasets that span different research objectives.

By grounding both manual and automated experimentation in shared vocabularies and schemas, we argue that this standardization is the most practical near-term step toward autonomous, data-driven electrochemistry.

POSTER #33

Martin Schmidt

Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM), Germany

Co-Authors: Martin Rudolph, Daniel Breite, Agnes Schulze

Data-driven design and functionalization of advanced polymer membranes

ABSTRACT

Polymer membranes are versatile materials for separation and purification applications in fields such as water treatment, food processing, and biomedicine. Their performance is determined by a complex interplay of material composition, processing conditions, surface chemistry, and mechanical properties. Data-driven approaches offer new opportunities to understand and optimize these relationships, enabling more efficient development of advanced membrane materials with tailored functionality.

This contribution presents data-driven strategies for the design and functionalization of polymer membranes. One focus is the biofunctionalization of porous membranes with different proteins and enzymes using a reagent-free electron beam irradiation method. Such modifications can improve membrane–biomolecule interactions and support the development of functional membrane systems for biotechnological and biomedical applications. By employing a design of experiments approach for predictive modeling, relevant processing parameters can be identified, their influence on functionalization efficiency can be evaluated, and optimized conditions can be proposed with reduced experimental effort. A second focus is the design and fabrication of advanced polymer membranes from recycled polymer materials or with functional particles integrated into the polymer matrix. Machine learning-assisted workflows can support the prediction of membrane properties from formulation and processing parameters, while uncertainty-aware optimization helps to identify promising candidate materials across multiple objectives.

Overall, the integration of experimental materials science with statistical and machine learning methods provides a powerful framework for accelerating materials development. By linking process parameters, material structure and properties, data-driven materials science enables a more targeted, resource-efficient, and adaptive design of advanced polymer membranes for novel sustainable applications.

POSTER #34

Anika Lorenz

NUWAM GmbH, Deutschland

Co-Authors: Uwe Scheithauer

Reinventing Chemical Processes: 3D-Printed High-Performance Ceramics for the Next Generation of Reactors and Mixers

ABSTRACT

NUWAM GmbH positions itself as an innovative technology provider in the rapidly growing market for additively manufactured high-performance ceramics. High-performance ceramics such as Al_2O_3 , ZrO_2 , SiC , and Si_3N_4 are characterized by outstanding chemical, thermal, and mechanical properties. By processing them using additive manufacturing technologies (3D printing), these properties can be incorporated into custom-designed reactors, mixers, and other components for applications in the chemical and process engineering industries, among others.

NUWAM, a company founded in the summer of 2025 and based in Radeberg near Dresden, Saxony, Germany, utilizes MPJ technology from D3-AM (Brixen, Italy), which combines high resolution with a large build volume ((480 x 400 x 180) mm³) and high productivity.

The founding team brings together decades of experience in application-oriented research in the field of additive manufacturing (AM) of high-performance ceramics and plant design, as well as product development and project management on an industrial scale. The combination of extensive experience and a broad network, coupled with the agility of a young company, makes NUWAM an ideal partner for businesses and research partners looking to break new ground or improve their processes.

During the presentation, we will use specific components (e.g., static mixers, heat exchangers, etc.) to demonstrate our current capabilities and discuss the challenges along the entire process chain that we are tackling together with our colleagues from D3-AM and the Fraunhofer IKTS in Dresden to further push the boundaries of what is possible.

POSTER #35

Gerhard Fröse

nanoSTAB, Germany

Polymer-Enhanced In-Place Cold Recycling Road Construction Technology - A Scalable Approach to Circular Construction Chemistry

ABSTRACT

Global road construction demands enormous quantities of materials. Approximately 300,000 km of new roads are built annually, while over 300 million km require renovation, representing a combined market of roughly USD 1.5 trillion per year. Conventional road construction relies on extraction of virgin aggregates, transport of bulk materials, and repeated asphalt application, a linear model with significant resource and emissions burdens. The disposal or replacement of existing road substrate represents one of the largest untapped recycling potentials in the built environment.

nanoSTAB® is a polymer-enhanced in-place cold recycling technology developed over 20 years of applied research and applied internationally. The process eliminates excavation and material transport entirely: the existing road substrate is treated on-site through a seven-step process: cement spreading, polymer injection, milling and mixing, compaction, grading, secondary compaction, and a reduced asphalt surface layer. The active ingredient is an environmentally neutral aqueous emulsion combining natural organic compounds with amorphous nanoparticles. Upon application, the nanoparticles accelerate cement hydration kinetics, increase structural density, reduce water absorption, and eliminate shrinkage cracking, while latex components provide long-term flexibility under dynamic load.

The technology directly operationalizes circular principles at road construction scale. By stabilizing and upgrading existing substrate rather than replacing it, nanoSTAB® eliminates the need for virgin gravel and sand extraction while reducing required asphalt volume by up to 50% and cement consumption by up to 30%. Lifecycle analysis of documented projects demonstrates a construction cost reduction of 42% per kilometer compared to conventional methods, a 98% reduction in maintenance costs over 15 years, and cumulative lifecycle cost savings of up to 70%. Construction time is reduced by a factor of three, with a corresponding reduction in site-related emissions.

A 2024 reference project in Bad Wörishofen, Germany documented a direct CO₂ reduction of 115 metric tons for a single project segment. Extrapolated to global road renovation volumes, the technology represents a potential reduction of approximately 130 million metric tons of CO₂ annually, alongside savings of up to 5 billion metric tons of sand and gravel and 30 million metric tons of bitumen per year. nanoSTAB® has been applied in international projects in Germany, Ethiopia (including a 10 km highway section to Mekele Airport), Kazakhstan, Paraguay, Libya a. o. These executed projects have proven the technology's performance across diverse climate zones, soil conditions and traffic load categories.

nanoSTAB® demonstrates that road construction, one of the most material-intensive sectors globally, can transition to a circular model through applied polymer chemistry. The technology offers a scalable pathway to eliminate virgin material dependency in road construction while simultaneously reducing costs, emissions, and construction timelines. nanoSTAB® highlights the chemical mechanism, key performance data, and a comparative lifecycle assessment against conventional construction methods.

POSTER #36

Sanjay Lama

Institute of Analytical Chemistry, Leipzig University, Germany

Co-Authors: Hannes Westphal, Simon Schmidt, Rico Warias, Tanja Gulder, Detlev Belder

An Automated Platform for Enzymatic Microreactor Optimization

ABSTRACT

The efficient use of biocatalysts, such as enzymes, is essential for achieving the goal of integrating eco-friendly chemistry into industrial processes, as they enable highly selective reactions under milder and greener conditions. Immobilizing these enzymes into miniaturized continuous reactors, such as microfluidic immobilized enzyme reactors (MIERs), can improve stability while simultaneously reducing the consumption of solvents, reagents, and most importantly, valuable biocatalytic material. However, operating multiple microreactors and systematically investigating reaction conditions rapidly increase experimental complexity, necessitating automated, standardized workflows that simplify reactor handling, improve reproducibility, and enable continuous analytical monitoring.

In this work, we present a novel microfluidic screening platform that combines microreactor technology, multi-reactor integration, and online HPLC-MS analysis in a sequential automated workflow. This system generates comprehensive datasets describing the performance of immobilized enzymes under continuous-flow operation. An automated sample feed facilitates the systematic investigation of different substrates and reaction parameters, while external valve control enables clean, contamination-free switching between individual MIERs. Downstream of the biocatalysis module, the reaction effluent is monitored via an integrated HPLC-ESI-MS unit, providing detailed qualitative and quantitative information on enzymatic biotransformations. Because the sampling frequency is constrained by the time required for complete chromatographic separation of reaction components, we also evaluated a miniaturized, modular chipLC system that reduced separation time to 2 minutes and reduced solvent consumption by over 80%. Thereby providing a faster, resource-efficient platform for screening enzymatic reactions with minimal biocatalyst usage while obtaining reliable, high-quality HPLC-MS data.

Beyond biocatalysis, the analytical platform presented here can be readily implemented for the low-consumption screening of a wide range of heterogeneous catalysts. Moreover, the information obtained provides a valuable foundation for scaling up or numbering up continuous processes.

POSTER #37

Rajarshi SinhaRoy

Universität Leipzig, Germany

Co-Authors: Georg Künze

MambaDiff: A Spatio-Temporal SE(3) Diffusion Framework for Protein Conformational Trajectory Modeling

ABSTRACT

Protein conformational dynamics is essential for understanding molecular recognition, allostery, and functional regulation, yet efficient modeling of protein motion from trajectory data remains challenging. Recent SE(3)-based diffusion models have shown promise for protein backbone and conformation generation, while selective state-space models such as Mamba-2 enable efficient modeling of long sequential information.

We present MambaDiff, a generative framework for learning protein conformational changes from molecular trajectory data. Rather than treating conformations as independent static structures, MambaDiff learns from short trajectory windows anchored to a reference protein structure. In this sense, it acts as a protein "world model": it maintains an internal representation of the current conformational state, updates this representation over time, and decodes it back into plausible protein backbone conformations. This allows the model to study not only individual structures, but also short transition-like paths between conformational states.

MambaDiff combines SE(3)-aware geometric modeling with spatial and temporal state-space modules. The geometric component helps preserve meaningful backbone structure, while the temporal component learns patterns of conformational change across trajectory frames. The framework is intended for generating and analyzing protein conformational ensembles, proposing plausible short structural transitions, and supporting downstream ranking of realistic conformations. More broadly, MambaDiff provides a foundation for dynamics-aware protein modeling, with future extensions toward guided sampling, energy-informed generation, and evaluation of thermodynamic or kinetic properties.

POSTER #38

Mikhail Kalinin

Chemistry Department, Martin-Luther-University Halle-Wittenberg, Germany

Co-Authors: Elena A. Kalinina; Dmitry I. Sharapa; Harald Maid; Alexandra Freidzon; Haleh Hashemi Haeri; Dariush Hinderberger; Robert Dinnebier; Alexander S. Oshchepkov; Konstantin Yu Amsharov

Carbon-based molecular diradicals: prospective qubit platforms for quantum computers

ABSTRACT

We investigate the Dibenzoterrylene (DBT) molecule as a promising platform for quantum information applications. In different solvents, DBT can adopt multiple conformations, each characterized by a distinct energetic landscape and a different propensity for triplet-state population. This solvent-dependent conformational switching provides a pathway to modulate the photophysical properties of the molecule and, in particular, to control access to triplet states relevant for spin-based quantum technologies. Our study highlights the relationship between molecular conformation, solvent environment, and triplet-state energetics, demonstrating the potential of DBT as a tunable material for qubit control.

POSTER #39

Immo Serbian

CovaSyn GmbH, Germany

Co-Authors: Oliver Kraft

From 14% to 92%: Deterministic Tool Orchestration for Chemistry-Capable AI Agents

ABSTRACT

Large language models are increasingly used as scientific assistants, yet on symbolically verifiable chemistry tasks they remain unreliable: in independent evaluation, frontier models answer correctly only 14-41% of the time. The failure mode is structural: probabilistic text generation is poorly suited to deterministic chemical computation. We present an alternative division of labour in which the language model acts not as a calculator but as an orchestrator of deterministic, domain-specific tools, exposed through the Model Context Protocol (MCP).

The platform provides more than 130 deterministic tools across 17 suites, spanning physicochemical property prediction, ADMET and toxicity screening (including ICH M7 mutagenicity), design of experiments and experiment optimization, stability and shelf-life modelling (ICH Q1), solubility and crystallization, retrosynthesis, docking, analytical-spectra interpretation (NMR, MS, IR, UV/Vis) and biologics design. Because each tool is deterministic, outputs are reproducible and auditable, a prerequisite for regulated chemistry and pharmaceutical work.

On the same independent benchmark (MolecularIQ, Klambauer Lab, JKU Linz; 3,540 verifiable tasks), connecting these tools raises model accuracy from 14-41% to 76-92%. We argue that this orchestration paradigm - probabilistic reasoning over deterministic computation - lowers the cost and barrier of computational assessment, supporting faster and more resource-efficient chemical research and drug discovery.

POSTER #40

Emin Açıkkalp

Eskisehir Technical University, Turkey

Co-Authors: Hurşit Değirmenci, Ali Günerhan, Önder Altuntaş, Jaroslaw Milewski

Methane Assisted CO₂ Co-Electrolysis and High Temperature Heat Pump Integration in Brewery Energy System for CO₂ Recycling and Decarbonization

ABSTRACT

In this study, a large-scale brewery plant is considered to improve energy efficiency and reduce CO₂ emissions. The CO₂ and wastewater generated during the brewing process are utilized in a Solid Oxide Electrolyzer (SOEC) for CO₂ co-electrolysis to produce syngas (H₂ and CO), which is subsequently used in the natural gas boiler to decrease fossil fuel consumption and associated emissions. In addition, low-temperature waste heat (~120 °C) is recovered and upgraded to 155 °C using a high-temperature heat pump (HTHP) to meet process heat demand.

The economic feasibility of the proposed integrated system is evaluated through the payback period (PP), while environmental benefits are assessed in terms of CO₂ emission reduction. Furthermore, a sensitivity analysis is conducted to identify the most influential parameters affecting system performance. The results show that the proposed system enables savings of 1181.64 t/year of natural gas and 337.50 t/year of CO₂ emissions, corresponding to an annual economic benefit of 281,030 €. The calculated payback period is 3.25 years, indicating a promising investment potential. The sensitivity analysis reveals that the electricity cost (ec) is the most critical parameter, exhibiting highly nonlinear behavior and significantly increasing system sensitivity at higher values, which may lead to unstable economic performance. In contrast, the natural gas cost (ngc) demonstrates a consistently negative sensitivity, indicating a stabilizing effect on the system. The carbon footprint of electricity (ecf) shows moderate sensitivity at low values but transitions into a highly sensitive regime beyond a threshold (~0.6–0.7), highlighting the importance of electricity source selection.

Overall, the results indicate that the proposed integration of SOEC and HTHP in brewery plants offers a technically and economically viable pathway for decarbonization, particularly under favorable electricity pricing and carbon intensity conditions.

POSTER #41

Onder Altuntas

Eskişehir Technical University, Turkey

TBA

ABSTRACT

TBA

POSTER #42

Zekiye Erarslan

CASUS, Germany

Co-Authors: Hossein Mirhosseini, Sascha Thinius, Laura König-Mattern, Thomas D. Kühne

Rational Design of Solvent Systems for Cellulose Dissolution: Integrating Machine Learning Potentials with Atomistic Simulations

ABSTRACT

The transition toward a circular bio-based economy requires efficient utilization of cellulose as a renewable feedstock for sustainable materials, textiles, and chemicals. Despite its abundance, cellulose remains difficult to process because of its extensive intermolecular hydrogen-bonding network, which makes dissolution a major challenge. Current industrial dissolution technologies often rely on environmentally hazardous solvents, while many greener alternatives remain poorly understood at the molecular level. Developing sustainable solvent systems, therefore, requires a detailed understanding of the interactions governing cellulose dissolution.

This project employs molecular dynamics (MD) simulations driven by state-of-the-art machine-learning interatomic potentials to investigate the molecular mechanisms underlying cellulose dissolution in ionic liquids. The simulations will quantify structural, energetic, and dynamical descriptors, including hydrogen-bonding networks, solvation structures, interaction energies, and conformational changes of cellulose. By correlating these molecular-level properties with solvent composition and experimentally observed dissolution behavior, this work aims to identify the key physicochemical factors governing solvent performance. The resulting framework will contribute to a predictive understanding of cellulose dissolution and support the rational development of environmentally benign solvent systems for sustainable biomass processing.

POSTER #43

Li Wan

Martin-Luther-Universität Halle-Wittenberg, Germany

Co-Authors: Mahdi Bagherpoor Helabad, Lena Fraedrich, Sarel J. Fleishman, Martin J. Weissenborn

Machine Learning directs htFuncLib from Mutational Compatibility to Substrate-specificity

ABSTRACT

Enzyme engineering for specific substrates and reactions is often constrained by the limited throughput of assays required to resolve activity, regioselectivity, and stereoselectivity. This challenge is particularly acute for unspecific peroxygenases, whose repurposing toward non-native substrates frequently requires coordinated active-site mutations but relies on chromatographic product analysis. Here, we report a machine-learning-guided htFuncLib workflow that converts compact, mutationally compatible combinatorial libraries into substrate-enriched libraries using experimentally assayed data. Benchmarking on four-position fitness landscapes of three proteins showed that the htFuncLib-ML strategy enriched high-fitness sequence spaces more efficiently than conventional stepwise directed evolution and can access productive multipoint variants missed by directed evolution. We then applied the workflow to engineer *Myceliophthora thermophila* unspecific peroxygenase (MthUPO) for selective γ -damascone hydroxylation. Screening and sequencing of 506 htFuncLib-derived designs identified 176 functionally secreted variants, of which 123 exceeded wild-type activity. ML-guided enrichment generated an activity-enriched library in which 90% of designs outperformed the wild type. The best variant, MthUPO_11C5, displayed a 5.1-fold activity increase, a turnover number of 1518, and >99% regioselectivity toward 4-hydroxy- γ -damascone. Molecular dynamics simulations indicate that these gains arise from reorganization of the substrate-binding cavity. This work establishes ML-directed htFuncLib as an efficient strategy for extracting substrate-specialized enzyme variants from experimentally tractable multipoint libraries under low-throughput screening constraints.

POSTER #44

CTC ACT (Academy for the Transformation of Chemistry)

Center for the Transformation of Chemistry, Germany

Co-Authors: Toni Grell, Juliane Adler, Markus Lange

Shaping Sciencepreneurs

ABSTRACT

Young researchers predominantly aspire to the academic career or join industry sooner or later after their PhD. Contrarily, entrepreneurship as a third career path is underrepresented, especially in Chemistry and related sciences. CTC as an innovation-driven research center will cultivate an entrepreneurial mindset among its early career researchers to empower them to transfer their results to application, thus bridging the gap between groundbreaking science and real-world impact. For this reason, all PhD candidates at the CTC will be educated and trained to become Sciencepreneurs.

Sciencepreneurs take research further – from scientific discovery to concrete solutions. Sciencepreneurs are scientists who publish their findings and transform them into marketable products, services or startups.

To achieve this ambitious goal, the CTC designs, organizes, and provides workshops and events that equip PhD candidates with the skills, competences, networks, and confidence to launch their own deep-tech ventures. Some formats will be developed and hold together with strategic collaborators like the Handelshochschule Leipzig or the Max-Planck Society.

POSTER #45

Mohammed Al-Yusufi

Fraunhofer Institute for Applied Polymer Research (IAP)

Co-Authors: D. Michalik, N. Steinfeldt, M. Sebek, H. Atia¹, R. Eckelt, C. Kubis, T. Murayama, T. Ishida, A. AbdelMageed, A. Köckritz¹

Continuous Transfer Hydrogenolysis of Furfural Derivatives to 1,5-Pentanediol (1,5-PDO) over Stable Nickel Catalysts: Toward Sustainable Synthesis of Renewable α,ω -Diols

ABSTRACT

α,ω -Diols are value-added monomers that are primarily produced from petrochemicals and are widely used for producing technical plastic, polyester and polyurethane resins.¹ Due to the associated plastics pollution with plastic materials, there is a high demand for the development of sustainable reaction routes for their synthesis from bio-based lignocellulose feedstocks. For instance, direct hydrogenolysis of tetrahydrofurfuryl alcohol (THFA) to 1,5-pentanediol (1,5-PDO) over Rh or Ir catalysts.² However, due to the high costs of these catalysts and their low stability in the continuous process,³ it is essential to replace them with stable nickel catalysts, which have more potential for large-scale industrial applications.

Continuous transfer hydrogenolysis (CTH) of THFA to 1,5-PDO was developed for the first time using stable Ni-La(OH)₃ catalysts in the H-donor isopropanol. Remarkably, 40Ni-La(OH)₃ was selective to 1,5-PDO (87%) and demonstrated high stability in long continuous runs (up to 386 h TOS).⁴ Following the evaluation of experimental and spectroscopic results, a direct hydride attack mechanism was proposed for the hydrogenolysis of the C–O bond of THFA on the interface between Ni and basic La(OH)₃ support. At this interface, the strong basic sites deprotonate the hydroxyl group of THFA, and metallic Ni species dehydrogenate isopropanol.⁵

References

1. P. Werle et al. "Alcohols, Polyhydric", Ullmann's Encyclopedia of Industrial Chemistry 2008, 1-18.
2. S. Koso et al. J. Catal. 2009, 267, 89-92.
3. B. Pholjaroen et al. T. Catal. Today 2015, 245, 93-99.
4. M. Al-Yusufi et al. A. ACS Sustain. Chem. Eng. 2022, 10, 4954-4968.
5. M. Al-Yusufi et al. ChemCatChem 2024, 16, e202400008.

POSTER #46

Tillmann Buttersack

Fritz-Haber-Institut

Direct observation of carbon dioxide uptake by amine solutions

ABSTRACT

Countering global warming requires active removal of carbon dioxide CO₂ from the atmosphere through capture technologies, since natural sequestration pathways, such as uptake by the oceans, vegetation, and soil, are not sufficient to offset anthropogenically-generated emissions. In the present study we directly investigated the uptake of CO₂ by amine solutions under atmospheric conditions. We used a combination of X-ray photoelectron spectroscopy and molecular dynamics simulations to demonstrate that the chemical composition in the interfacial region during CO₂ uptake strongly differs from that in the bulk at any level of CO₂ saturation. The measurements allow us to directly determine the apparent pH of the nanometer-thin interfacial region during CO₂ uptake, indicating differences in the mechanism for carbamate formation at the liquid-vapor interface compared to the mechanism in the bulk of the solution. Our study directly probes the interfacial CO₂ capture mechanisms under non-equilibrium conditions that resemble those in real-world carbon capture technologies.

POSTER #47

CTC DECO (Data Engineering and Computation)

Center for the Transformation of Chemistry, Germany

Co-Authors: Lenz Fiedler, Mayank Agarwal, Yasmine Ben Ameer, Surya Teja Pathakoti, Valentina Vendittoli

Open source research data infrastructure for a modern chemical research center

ABSTRACT

Chemical research suffers from a well-documented data gap. While immense amounts of research data are created globally every day, they are often inaccessible to data-driven methods, be it for technological or conceptual reasons. The Center for the Transformation of Chemistry seeks to close this gap by integrating its chemical research facilities with a comprehensive data infrastructure that creates AI-ready data datasets to tackle pressing research topics concerning a circular chemical economy. Shown here is an overview of the current development efforts in this regard, in the form of the open-source python package "Collection of Tools for Scalable data Extraction and pipeline Automation" (CTSEA).

POSTER #48

Robert Röllig

BioEconomy e.V.

Co-Authors: Dr. Andrea Weißel, Robert Röllig, Lisa Plümer, Hem Dipakbhai Thothawala¹, Felix Schwarzenberger, Mario Sternberg, Prof. Dr. Thomas Kirschstein¹

Central Germany's Chemical Industry 2035 – Transforming the Feedstock Base

ABSTRACT

The Central German chemical industry is one of Germany's largest integrated production regions, linking the industrial sites of Böhlen, Schkopau, Leuna, Bitterfeld-Wolfen, Piesteritz and Zeitz through highly interconnected infrastructure, feedstock and product flows. The planned closure of Dow Chemical's Böhlen steam cracker by the end of 2027 represents a major structural challenge, as downstream value chains will lose a primary source of petrochemical feedstocks.

This study provides the first systematic assessment of future feedstock supply options, biomass and CO₂, for the region after the cracker closure. Existing material flows were analyzed, three transformation pathways were developed, and their feedstock, energy and infrastructure requirements were comparatively evaluated.

The results show that no single pathway can fully replace today's petrochemical production system under current conditions. Instead, the long-term competitiveness of the region will depend on exploiting regional strengths in feedstock potential, expanding renewable energy infrastructures, and establishing new cross-sectoral value chains. The study offers practical recommendations as well, concluding that the feedstock transition requires not only technological innovation but also closer integration of the chemical industry with the energy, agricultural, forestry and waste management sectors.

POSTER #49

Dr. Clement Owusu Prempeh

DFBZ

Co-Authors: Ingo Hartmann, Steffi Formann, Manfred Eiden, Katja Neubauer, Hanan Atia, Alexander Wotzka, Sebastian Wohlrab, and Michael Nelles

Performance and characterization of Sol-Gel-Derived Cornhusk Support for Low-Temperature Catalytic Methane Combustion

ABSTRACT

This study investigates the performance and characterization of sol-gel derived cornhusk support for low-temperature methane combustion (LTCCM) using palladium-ceria (Pd/CeO₂) catalysts. The cornhusk support was prepared using a sol-gel method and characterized using various techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and N₂ physisorption. The prepared cornhusk support catalyst (Pd/CeO₂/CHSiO₂) was tested for LTCCM, and its performance was compared with a commercial catalyst (Pd/CeO₂/commercial). The results showed that the Pd/CeO₂/CHSiO₂ catalyst exhibited higher catalytic activity than the commercial catalyst at low temperatures, with a conversion of 50% at 394 °C compared with 593 °C for the Pd/CeO₂/commercial. The superior performance of the Pd/CeO₂/cornhusk catalyst was attributed to the highly dispersed Pd/CeO₂ nanoparticles on the cornhusk support, which provided a bimodal pore system and enhanced the reducibility of PdO. Overall, this study suggests that sol-gel-derived cornhusk support has the potential to be a promising alternative support for LTCCM catalysts.

POSTER #50

Robin Tannert

University of Applied Sciences Zittau/Görlitz

Co-Authors: Florian Praße, Daniel Fischbach, Jens Weber

Lignin-Based Thermosets: Challenges and Opportunities in the Manufacturing of Renewable Polymers

ABSTRACT

Furthermore, the inherent structural heterogeneity of lignin, originating from both botanical source and extraction process, significantly influences polymer synthesis, material properties, and processing behavior. These results highlight both the opportunities and limitations of lignin as a renewable feedstock and underline the importance of evaluating industrial feasibility alongside sustainability when developing next-generation bio-based thermosets. We will discuss our learnings on the necessity to bridge scales from lab to production.