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Faculty of Technical Chemistry, Chemical and Process Engineering, and Biotechnology

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Book of Abstracts for Posters

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Structure-guided investigation of parameters determining enzyme-catalyzed reactions

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Enzymes play an indispensable role in all molecular processes in life. Their substrate and regio-specificity are embedded in their three-dimensional structure. In addition, the structure also con-tains information on the biochemical reaction to be performed on the substrate. Thus, knowing the three-dimensional structure paves the way to a deeper understanding of enzyme properties. Equal-ly important are kinetic and thermodynamic parameters in the study of enzyme reaction mecha-nisms. Therefore, in our research, we integrate these different aspects of enzymology to better understand enzyme reaction mechanisms in order to make enzymes amenable to biocatalysis and drug discovery. Toward these aims, we employ a multidisciplinary approach encompassing kinetic, thermodynamic, spectroscopic, and structural techniques (Figure 1).

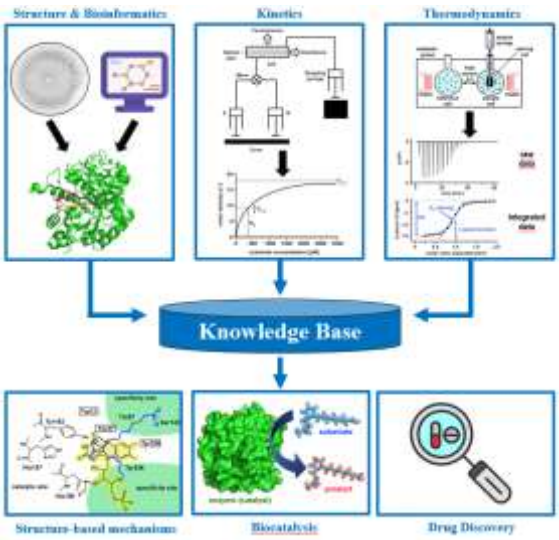

Figure 1: Scheme of our research approach.

Envisaged internal collaborations

Our institute will collaborate with the Institute of Organic Chemistry (Breinbauer group), which will synthesize substrates, coenzyme analogs, and inhibitors. These compounds are needed to shed light on enzyme-catalyzed mechanisms and to develop potential drug candidates targeting specific enzymes.

Furthermore, we will collaborate with the Institute of Molecular Biotechnology (Kourist Group) to assess the potential of enzymes as valuable biocatalysts. For this purpose, we will kinetically characterize promising biocatalysts, providing information about their activity and substrate and reaction scope

Disease suppression through plant and soil microbiome diversity

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Abstract

Plant seeds harbour distinctive microbiomes that interact with complex soil microbial communities throughout development, fundamentally shaping plant health, and resistance to soil-borne diseases. Seed-associated microbial communities undergo dynamic changes influenced by nutrient availability and soil conditions, while the soil microbiome diversity plays a pivotal role in mediating plant growth promotion and pathogen suppression. Our projects aim to investigate how organic amendments and novel substrates, sourced from organic agricultural residues, can be leveraged to manage soil and plant microbiome composition and functionality. Drawing on evidence that humic substances from hydrothermal humification and compost-derived amendments stimulate recruitment of disease-suppressive bacterial assemblages, we are developing next-generation substrates and seed coatings by incorporating beneficial microbial consortia designed to enhance plant performance and systemic resistance. Focusing on tomato production systems, we integrate organic soil amendments with microbiological interventions to reduce agrochemical dependency. Our approach exploits natural microbial interactions including rhizobacterial interactions that promote plant health to foster resilient cropping systems while countering soil degradation in alignment with circular bioeconomy principles.

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Envisaged internal collaborations

Potential internal collaborations can be envisaged to integrate biobased materials and sustainable chemical processes into microbiome management strategies. These partnerships could enhance the development of eco-friendly substrates and seed coatings by combining expertise in biotechnology, chemical engineering, and environmental science. Collaborative efforts could support the identification, cultivation, and application of beneficial microbial consortia.

Flowing Power: Design, Synthesis and Characterization of Water-Soluble Phenazines in Redox-Flow Batteries

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Through the emergence of solar and wind power, a larger urgency for long term energy storage arises when power generation is absent through lack of sun and wind.[1] One emerging technology to tackle this issue are redox-flow batteries (RFBs).[1,2] While organic solvents may be used in RFBs, water has a distinct advantage in terms of cost, safety, and environmental impact. To maximize energy density, redox-active molecules for aqueous RFBs should be designed to offer high solubility in water and high chemical stability.[3,4] Phenazines are a promising family of organic molecules for aqueous RFBs offering high chemical stability and energy density and have already been utilized in RFBs.[5]

We have designed and synthesized several new water-soluble phenazines. Starting with a stepwise Wohl-Aue reaction, the phenazine core structure was successfully synthesized. The bromine handle offers a unique opportunity for further functionalization through Mizoroki-Heck reaction as well as Negishi cross-coupling to access a variety of functionalized phenazines bearing water-solubilizing groups. These new compounds were evaluated for their redox potential as well as life-cycle stability in aqueous RFBs.

Envisaged internal collaborations

None.

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Optical control of phosphatase activity in naturally occurring red-light regulated PPM phosphatases

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Protein phosphorylation is an essential posttranslational modification involved in numerous cellular processes. Metal-dependent protein phosphatases (PPMs) in particular comprise a conserved catalytic core domain that can be linked to a variety of unique N- or C-terminal regulatory modules [1]. In bacteria, one particular subgroup of sensors that occurs linked to a PPM output module (OPM) are red light-sensitive photoreceptors termed “phytochromes” featuring a PAS-GAF-PHY domain architecture [2]. Much like PPMs, bacterial phytochromes (BphPs) are modular components naturally linked to a range of effector domains and capable of integrating light signals via diverse OPMs. In the context of protein phosphorylation, we are characterising PPM-linked phytochromes (PpmPs) with regards to their spectral as well as functional properties. PPM phosphatases play a key role in regulation of bacterial gene expression by affecting protein-protein-interactions (PPI) in the form of sigma factor/anti-sigma factor/anti-sigma factor antagonist (ASA) partner-switching. The representative PPM-linked phytochrome *Np*PpmP has shown light-controlled modulation of dephosphorylation of its physiological ASA substrate in mass spectrometry (MS)-based analyses. Future efforts will include detailed probing of enzymatic activity on the substrate ASAs *in vitro*, and *in vivo* investigation of light effects on gene expression using transcriptomics. Appreciating the dynamic range of these optically controlled phosphatases and the molecular requirements for sensor-effector integration will open up new avenues for optogenetic control of similar phosphatases. The many essential biological mechanisms involving (de)phosphorylation especially constitute an intriguing basis for the development of novel optogenetic tools [3].

Envisaged internal collaborations

Mass spectrometry-based protein analytics – covalent protein modifications (intact mass analysis), protein-protein interactions and ligand binding (native mass analysis), protein dynamics (hydrogen-deuterium exchange coupled to MS)

Protein-protein interactions – chemical modification of the phosphorylated substrate protein (PPI strengthened if hydrolysis is impossible?)

Transcriptomics analyses of PpmP-carrying bacterial systems comparing the effect of (far-)red light under different stress conditions

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Native chemical ligation (NCL) of peptides to polysaccharides: an in situ ^{1}H NMR study

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Native chemical ligation (NCL) refers to the well-known formation of an amide bond between a C-terminal thioester and an N-terminal cysteine of peptides or proteins.[1] High chemoselectivity, complete avoidance of protective groups on amino acid residues and compatibility with aqueous, physiological conditions make NCL a biologically benign and effective method for synthesis of polysaccharide-peptide conjugates, which are becoming increasingly pivotal in the development of targeted drug delivery systems, vaccines and tissue engineering scaffolds.[2,3] Our work introduces in situ, real-time monitoring of a highly robust, peptide-to-polysaccharide NCL method. The peptide is ultimately ligated to the polymer solely through stable amino acid-based amide bonds under aqueous, pH-neutral conditions without any exogenous and potentially problematic linker molecules.

Envisaged internal collaborations

Incorporation of bioactive molecules (e.g. drugs, peptides, proteins, etc.) into our polysaccharide material platforms; Biological testing (cell viability, growth/proliferation, biological response).

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Zeolitic Imidazolate Framework-Based Biocomposites: Semi-automated Synthesis and Interactive Visualization

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Zeolitic imidazolate framework (ZIF) biocomposites integrate the diverse bioactivities of biomacromolecule encapsulation with the stability and tunability of metal–organic frameworks[1][1] and are widely studied for their potential in biocatalysis and biomedicine. However, their preparation is highly sensitive to precursor composition, concentration, washing conditions, and operator-dependent handling procedures.[2,3] This sensitivity is reflected in the diverse products that can form from the same precursors under different synthesis and processing conditions, including sodalite (**sod**), diamondoid (**dia**), katsenite (**kat**), **ZIF-L**, **ZIF-C**, **ZIF-EC-1**, amorphous materials, highly defective phases, or combinations thereof.[2] Here, we combine semi-automated syringe-pump synthesis with interactive visualization to map synthesis–structure–property relationships in ZIF biocomposites. A programmable four-syringe pump platform was used to systematically prepare 360 synthesis conditions in triplicate (1080 samples in total). The investigated synthetic parameters were the concentrations of metal, ligand, and protein, their relative amounts, total precursor concentration, and washing protocol. Structural, chemical, and functional characterization yielded a dataset of ~2250 entries comprising crystalline-to-amorphous ratios, IR-based protein-to-framework ratios, encapsulation efficiency (EE%), and loading capacity (LC%). We note that exploring such a large dataset manually can be troublesome and that current static visualizations can hide meaningful trends.[2] With the aim of enabling customized and interactive exploration of the data, we designed the ZIF Biocomposite Explorer App (ZIF-BEA), which supports user-defined navigation, providing direct access to experimental data and trends on material properties. We anticipate that integrating large experimental datasets with interactive digital visualizaton may expedite the design of MOF biocomposites, while providing a tool for the exploration of other classes of functional materials.

Envisaged internal collaborations

The further development of this research will be supported by collaborations within the TCVB Faculty, especially through the TU Graz Lead Project Porous Materials @ Work for Sustainability (PMWS, LP-03). The project can benefit from complementary expertise in porous materials, analytical chemistry, biotechnology, and data visualization.

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Polyvalent Ligand Presentation on Click-Functionalized Cellulose

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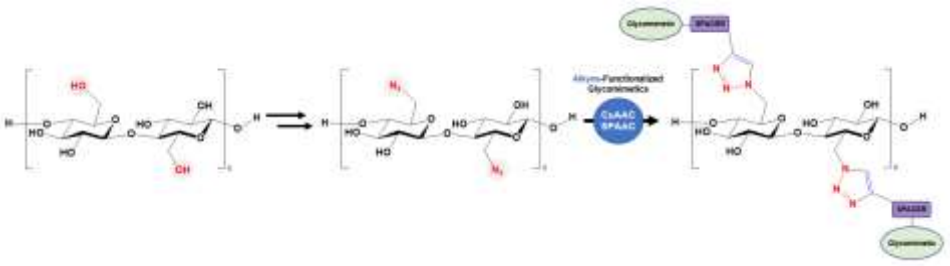
Multivalent interactions are central to biological recognition, where simultaneous interaction of multiple carbohydrates with respective lectins enhances affinity and selectivity via the cluster glycoside effect [1]. In this respect, polysaccharides such as cellulose and chitosan can serve as abundant, biocompatible, and chemically accessible scaffolds for the dense, controlled polyvalent display of bioactive ligands [2–4].

In this work, we present concise, efficient synthetic routes to polyvalent, polysaccharide-based systems. Synthetic bioactive small molecules (glycomimetics), including lectin antagonists and glycosidase inhibitors, are covalently coupled to cellulose using copper-catalyzed azide-alkyne cycloaddition (CuAAC) and copper-free strain-promoted azide–alkyne cycloaddition (SPAAC) [2,4,5] (Scheme 1).



Scheme 1: Synthetic strategy for the generation of polyvalent cellulose-based systems.

These modular functionalizations provide precise control over ligand density and spatial arrangement, amplifying binding strength and stability through multivalent effects and enabling application-tailored interfaces for biomedical use [2,4,5].

Experimental details and biological evaluation will be presented.

Envisaged internal collaborations

For in-depth structural characterisation, advanced NMR spectra are measured by Hansjörg Weber from the Institute of Organic Chemistry (TCVB). Infrared Spectroscopy, as well as, DLS measurements are performed in cooperation with the Institute of Inorganic Chemistry (TCVB).

Financial support: Austrian Research Foundation FWF, Weave Austria - Prague PIN 5558524 and the Czech Science Foundation (25 – 18949L) and WTZ (OeAD: MULT 01/2025 and Cz: 8x25048).

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Using *in-situ* and *operando* X-ray powder diffraction and ^{7}Li NMR to monitor solid-state reactions in batteries

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NMR spectroscopy and X-ray powder diffraction are both contact-free methods capable of probing closed electrochemical systems and providing valuable insight into solid-state reactions in batteries. *Operando* ^{7}Li NMR is highly sensitive to changes in the local environment and can detect even small amounts of lithium plating, while also offering information on short-range structure and ion dynamics [1]. In contrast, XRPD provides time-resolved access to long-range order and solid-solid phase transitions that govern voltage profiles in Li-ion cells [2]. Using both techniques independently highlights their complementary strengths and demonstrates how local and long-range probes together deepen our understanding of electrochemical solid-state processes during operation.

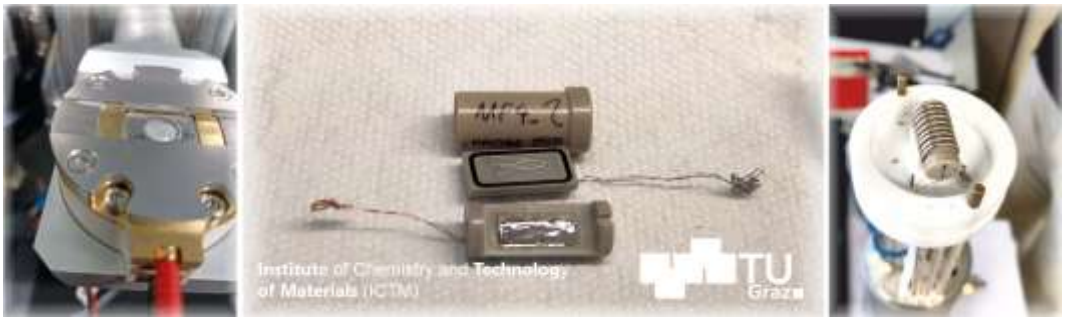

Figure 1: Typical lithium-ion battery active materials react with components of the ambient atmosphere and must therefore be handled under inert-gas conditions. Specialized sample holders are required to enable electrochemical reactions while remaining compatible with *in-situ* measurements. A coin cell sealed with a 20 µm thin Al current collector that also serves as an X-ray transparent window for monitoring phase changes during reaction progress (left). A metal-free cell housing designed for NMR measurements and fitting into the coil of a dedicated NMR probe is shown in the middle and right panels.

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Fast Li^+ Diffusion in Lithiated LATP as Seen by Motion-Induced Nuclear Spin Relaxation

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Lithium aluminum titanium phosphate (LATP) is well-established as a crystalline electrolyte offering fast Li^+ diffusion pathways. However, when in contact with lithium metal, LATP forms a mixed-conducting interphase, potentially impacting the performance of LATP-based batteries [1, 2]. During lithiation,Ti^{4+} is partially reduced to form Ti^{3+}, and Li^+ occupies vacant sites within the NaSICON-type structure. In this study, we employed ^7Li NMR to investigate changes in Li^+ diffusivity induced by chemical lithiation using *n*-butyllithium. Chemical lithiation via a single electron transfer reaction allowed us to mimic the structural and dynamic changes occurring within a lithium metal battery. Our findings reveal that lithiation does not hinder Li diffusivity; rather, ^7Li NMR relaxation measurements indicate enhanced local hopping processes, which may facilitate improved long-range ion transport [3]. Despite the formation of a lithiated interfacial layer that propagates inward, the dynamic properties of LATP remain resilient. These results highlight that the electrochemical degradation process does not compromise the intrinsic ion transport properties of LATP.

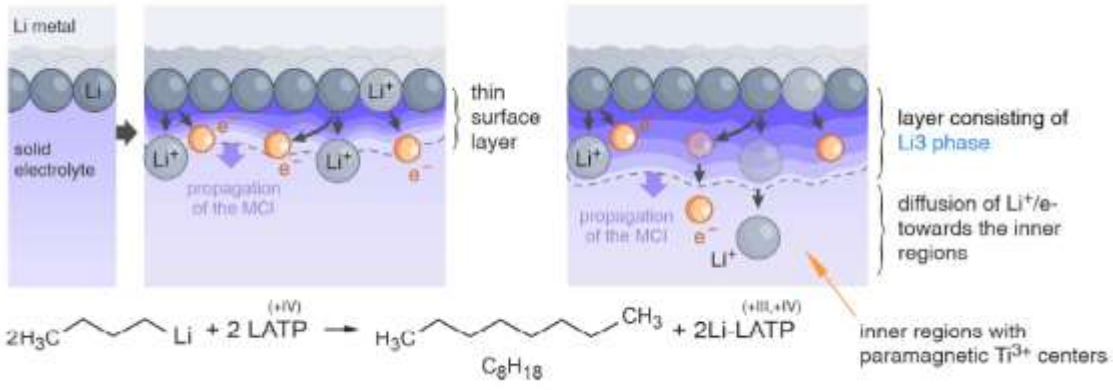

Figure 1: Lithiation of LATP upon contact with metallic Li^0. The propagation of a mixed-conducting degradation layer into the interior of an LATP particle is illustrated. At sufficiently high lithiation levels, the Li_3 phase forms.

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Analytical Chemistry and Food Safety: From Genotoxicity to Sensory Relevance

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Analytical chemistry has traditionally focused on the identification and quantification of chemical constituents in samples of interest. Today, however, we are increasingly confronted with the challenge of understanding highly complex chemical mixtures relevant to food safety, quality, and sensory properties. Conventional single-substance analysis is reaching its limits, while modern instrumentation enables highly detailed profiling of ultra-trace compounds. Yet, the biological and sensory relevance of these measurements often remains unclear. This gap highlights the need to rethink the role of analytical chemistry in food safety: it is not merely a tool for measurement, but an integral part of a broader, effect-oriented understanding of complex mixtures. In this context, analytical chemistry plays a central role, although its impact increasingly depends on close integration with toxicology, bioanalytics, and sensory science. Addressing the relationship between chemical composition and functional outcomes is therefore inherently interdisciplinary and represents a major research focus of the “Food Safety” working group at the Institute of Analytical Chemistry and Food Chemistry.

This poster uses post-consumer recycled (PCR) polyolefins intended for future food-contact applications according to current EU legislations to demonstrate the role of modern analytical chemistry. PCR polyolefins often exhibit highly complex chemical compositions that cannot be adequately described using single-compound strategies alone. Advanced instrumental techniques such as comprehensive two-dimensional gas chromatography (GC×GC) provide detailed chemical profiles which, within the FFG collective research project “Aurelia”, are combined with Ames MPF assays to investigate biological effects such as genotoxicity, and with sensory science approaches to evaluate material-related (off-)odor profiles in an interdisciplinary framework. Using this integrated approach, several critical alert factors for polyolefin recycling have already been identified, underlining the essential role of analytical chemistry in modern food safety assessment.

Envisaged internal collaborations

Established collaborations with the Institute of Bioproducts and Paper Technology focus on the safety assessment of fibre-based packaging materials. More broadly, our research addresses challenges related to the circular economy, including recycling, re-use, renewable resources, and the associated implications for product quality and safety. By combining advanced hyphenated and multidimensional chromatographic techniques with automated sample preparation, we develop interdisciplinary analytical approaches that support effect-oriented characterization of complex mixtures. These methods enable investigation of the sources and formation of undesired compounds and can be applied to diverse matrices and applications, including recycled materials, fibre-based products, (waste)water, soil, air analysis, process monitoring, and characterization of bio-based products.

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Discovery of non canonical phospholipid synthesis pathways utilizing ^{13}C-labelled glycerophosphate derivatives

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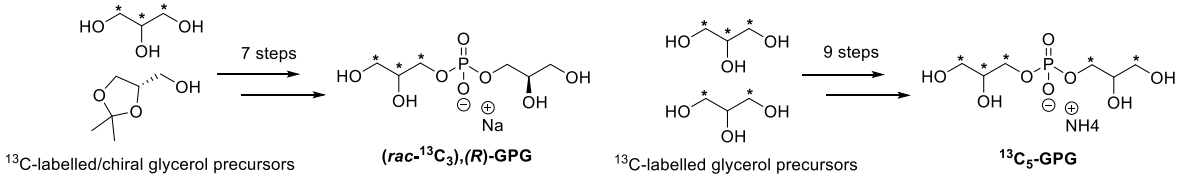
According to text book knowledge, *de novo* glycerophospholipid (GPL) synthesis begins with the acylation of glycerol-3-phosphate to form phosphatidic acid, the precursor of all other GPLs. New assymetrically ^{13}C-labelled derivatives of glycerophosphoglycerol (GPG) were synthesized as chemical probes (Scheme 1) and used in the discovery of an alternative GPL synthesis pathway that starts with the acyl-CoA-dependent acylation of GPG, resulting in the formation of lysophosphatidylglycerol (LPG).



Scheme 2: Assymetrically ^{13}C-labelled GPG derivatives synthesized for mass-spectrometry experiments.

The acyltransferase reaction is catalyzed by the Batten disease-associated protein ceroid lipofuscinosis neuronal 8 (CLN8). *CLN8*-knockout cells and mice cannot utilize GPG for BMP synthesis, resulting in BMP-deficiency and excess accumulation of phospholipids in lysosomes. The newly discovered lipid synthesis pathway is relevant for understanding lysosomal lipid metabolism and the pathogenesis of neurodegenerative diseases. BMP-deficiency may contribute to or even underlie lysosomal cargo accumulation in certain forms of Batten disease and other lysosomal storage disorders.

Envisaged internal collaborations

None, its already a collaboration

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Biocatalytic Exploitation of Enzymes Encoded in Glycoside Utilization Loci

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Recently, a novel non-hydrolytic pathway for degrading glycosides was discovered in bacterial glycoside utilization loci (GULs).[1,2,3] Unlike traditional glycosyl hydrolases, which are often limited by high substrate specificity, this pathway allows microbes to process a broader range of sugars by breaking down catalysis into manageable steps: oxidation at the C3 position, eliminative cleavage of the glycosidic bond, hydration, and finally a reduction at C3 position. While the enzymes encoded by these GULs have been well-characterized structurally and mechanistically, their potential for biocatalysis remains largely underexplored.

In this work, we present a panel of keto-glucosides synthesized using two enzymes originating from GULs. First, we utilized an unusually promiscuous FAD-dependent glucoside-3-dehydrogenase from the *Rhizobium sp.* GUL.[3] We demonstrate that this enzyme is active on a diverse range of mono-, di-, and oligosaccharides accepting substrates with various glycosidic linkages (*O*, *C*, and *S*). By coupling this dehydrogenase with a laccase/ABTS system to facilitate FAD cofactor regeneration, we developed an efficient enzymatic cascade capable of producing 3-keto-glucosides on a gram scale. Furthermore, we demonstrate the usage of a *C*-glycoside eliminase from the human intestinal bacterium PUE GUL[3,4], to synthesize the *C*-glycoside 3-keto-nothofagin. The enzyme catalyses a 1,4-Michael addition between the glycosyl donor 2-hydroxy-3-keto-glucal and the aglycon phloretin by activating the aglycone to act as a nucleophile. This unprecedented reaction mechanism of CGEs can for the first time be utilized for *C*-glycoside synthesis.

Together, these enzymes demonstrate significant biocatalytic potential for the production of keto-glucosides, which can serve as versatile building blocks for rare sugars, novel polymers, and prebiotics.

Internal collaborations

The ongoing research on the human intestinal bacterium PUE GUL is being conducted in collaboration with Prof. Gustav Oberdorfer for structural analysis, and Prof. Hansjörg Weber and Prof. Rolf Breinbauer for product analyses using NMR and MS techniques.

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ToFuel - an integrated biorefinery for sustainable aviation fuel production from tomato residues

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The production of Sustainable Aviation Fuels (SAF) from renewable feedstock, such as agricultural waste streams, is vital in reducing the carbon footprint of the aviation sector and achieving the European climate neutrality goals. The ToFuel project focuses on converting waste streams from tomato production and processing into SAF, animal feed, fertiliser and nutritional oil via an innovative, efficient biorefinery concept. The innovative biorefinery concept efficiently processes a variety of feedstock, including agricultural residues and organic waste, to produce SAF. Addressing key challenges in biorefining- such as low product concentrations and complex, variable input streams, and water management, all of which contribute to high energy demand- the ToFuel project aims to develop advanced, integrated CO2-neutral SAF production technologies. The overall process includes biomass fractionation via extrusion and hydrothermal liquefaction, carbon capture using algae cultivation, microbial lipid fermentation on both liquid and solid media, the pre-concentration and purification of process streams by developing and adapting new technologies, and the upgrade to SAF via the HEFA route, to achieve cost parity with other biofuels.

The project will provide open-access models for process simulation, (social) life-cycle assessments, and life-cycle cost calculations, along with strategies for scale up. By project completion, the core technologies will reach TRL 5, ensuring industrial readiness. A major outcome of the project is an expanded knowledge of biorefinery, water management strategies, and carbon capture and utilization via algae, thereby reducing fossil resource dependency, strengthen Europe's leadership in sustainable fuel technologies and contributing to new green job creation. The ToFuel project will maximize impact through a clear communication and dissemination strategy, including stakeholder workshops at European and local levels, along with accompanying exploitation measures.

Envisaged internal collaborations

Potential collaborations with ACIB or Institute of Bioprocess Engineering, Analytical Chemistry or working group Continuous Processes (IPPE).

Advancing Electrochemical Hydrogen Production: Diagnosis and Alternative Pathways

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Electrochemical hydrogen production is gaining momentum as a key pillar of the clean energy transition, with proton exchange membrane water electrolysis (PEMWE) as a leading technology and alternative electrochemical pathways emerging as promising complements. Despite significant efforts toward harmonization in PEMWE, variations in testing protocols, conditioning procedures, characterization methods, and reported metrics continue to hinder comparability across studies.[1], [2], [3] This challenge extends to the need for reliable and comprehensive membrane degradation metrics with increasing regulatory pressure on per- and polyfluoroalkyl substances (PFAS) in the EU. [4] In parallel, alternative electrochemical routes; such as sulphur dioxide electrolysis (SDE), offer potential advantages in energy efficiency by coupling hydrogen production to industrial processes, yet remain comparatively underexplored in terms of systematic characterization.

Here, we address both dimensions: we propose the initial open circuit voltage (OCV) response as an accessible membrane degradation metric for PEMWE to assess material suitability, enabling early identification of instability and performance variability without the need for extended durability testing. In addition, fluoride emission is commonly used to assess ionomer and membrane degradation, however, inconsistent trends across studies limit its interpretability and comparability. In this study we compare fluoride and total fluorinated compound measurements in PEMWE using two analytical techniques to provide a more comprehensive understanding of degradation pathways and products.[5]

On the alternative approaches to electrochemical H_2 production, we investigate SDE as an H_2 production pathway, evaluating its electrochemical performance, component optimisation and viability.[6] By modifying the catalyst from platinum to gold, the achieved performance is increased by ~30% while reducing critical raw material usage by 50% reaching energy consumption of 36.1 kWh/kgH_2. Using SAXS analysis of the PEM and the catalyst layer, it is revealed that under ultra-low loading (<0.1 mg/cm^2) of gold, Au-S crystals are formed, hindering the catalytic activity of the cell, effect not observed at loading above 0.1 mg/cm^2. These results provide a step forward in the understanding and future development of SDE as an alternative approach to achieve the hydrogen energetic transition.

Acknowledgement

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Microbiome Engineering for Sustainable Ecosystems and Agriculture

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Microbiomes form the invisible infrastructure of life on Earth, governing ecosystem stability, agricultural productivity, food quality, and environmental resilience. Our research develops microbiome-based biotechnological solutions for sustainable food production systems. We investigate microbiomes across interconnected agricultural and environmental systems, from soils and plants to post-harvest environments, storage, processing, and transport, to understand and engineer microbial functions along the entire production chain. Our technological approaches include synthetic microbial consortia, encapsulated beneficial microorganisms (BFC Technology, PCT/EP2018/075760), and plant–microbiome co-breeding strategies designed to enhance nutrient cycling, soil fertility, crop quality, food safety, and resistance against pathogens and abiotic stress while reducing dependence on chemical fertilizers and pesticides. Beyond agriculture, we investigate microbiome-driven strategies for biodiversity conservation, ecological restoration, and the renaturation of degraded ecosystems under increasing environmental and climate pressures.

Envisaged internal collaborations

Joint projects with colleagues specializing in protein expression and enzyme design could support the development of engineered microbial consortia for sustainable agricultural and environmental applications. Collaborative research may further address the combined effects of biological and chemical factors, including metal–microbe interactions (e.g., copper), and their impact on nutrient cycling, greenhouse gas emissions, and pollutant degradation. The development of biodegradable delivery systems or matrices for the controlled release of microbial consortia would also be a valuable area of research. The integration of metagenomic and metatranscriptomic approaches to unravel functional interactions and division of labor within complex microbial communities relevant to environmental remediation and waste valorization.

Computational Design of Sequence-Specific Metalloproteases for Scarless Affinity Tag Removal

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Current strategies for recombinant protein purification often rely on the use of affinity tags. However, scarless removal of affinity tags for downstream processes with proteases remains a major challenge. Using state-of-the-art de novo computational design tools, we engineered sequence-specific Zn-dependent metalloproteases to achieve precise cleavage and scarless affinity tag removal.

Top candidates from the computational protease design pipeline were selected via in silico scoring followed by experimental screening using a rapid, sensitive green fluorogenic GFP complementation assay.

Our approach enables the rapid development of sequence-specific proteases capable of cleaving custom affinity tags with high precision, with broad applications in recombinant protein production for biopharmaceuticals, biosimilars, and structural and functional studies.

Integrated gas fermentation: From microbial CO2 utilization to scale-up

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Gas fermentation enables the conversion of CO_2 and gaseous substrates into biomass and value-added products using autotrophic microorganisms. Current research at Graz University of Technology and acib combines microbiology, cell engineering, bioprocess engineering, automation and simulation approaches to develop scalable gas fermentation platforms. Experimental work focuses on explosion-proof small-scale reactor systems for the cultivation and characterization of hydrogen-oxidizing bacteria[1]. The investigated microorganisms are the well-known workhorse *Cupriavidus necator*, including native and engineered strains[2], as well as less-studied hydrogen-oxidizing bacteria that might be developed into alternative hosts.

As part of the DigiBioTech Lead project, experimental gas fermentation is combined with hybrid modelling, CFD simulations and machine-learning-assisted compartment modelling[3] to support reactor optimization and scale-up. The research further investigates metabolically engineered strains under mixotrophic conditions and the production of polyhydroxyalkanoates (PHAs) with improved material properties. Interdisciplinary collaborations contribute to the development of robust CO_2-based bioprocesses with strong industrial implementation potential.

Current internal collaborations

The collaboration with the Institute of Molecular Biotechnology on strain engineering of autotrophic microorganisms is a long-standing partnership within the TCVB Faculty. More recently, cooperation with the Institute of Process and Particle Engineering (IPPE) has expanded the research toward CFD simulations and reactor scale-up design. Established collaborations within other faculties of the university include the Institute of Automation and Control, supporting process automation and control strategies, and the Institute of Thermal Engineering, contributing to reactor design, safety, and gas handling.

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Li Jump Diffusion and Long-Range Transport in Garnet Single Crystals: Spanning the kHz−GHz Range

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Understanding Li-ion transport in garnet-type oxides is essential for solid-state electrolytes. Using single-crystalline $Li_{6.5}La_3Zr_{1.5}Ta_{0.5}O_{12}$, we probe Li dynamics from kHz to GHz via ^{7}Li NMR relaxation and conductivity spectroscopy. Long-range transport shows activation energies of 0.41 to 0.47 eV, while local dynamics yield approximately 0.22 eV [1]. Compared to $Li_6La_3ZrTaO_{12}$ [2], higher Li mobility is partially compensated by a lower effective charge-carrier concentration, making N_c a key parameter governing ionic conductivity.

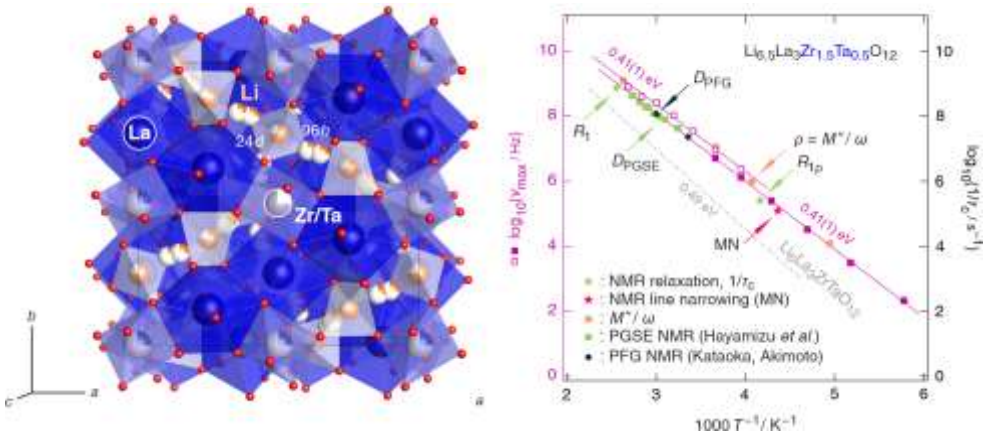

Figure 1: Crystal structure of Li-bearing garnet oxides and characteristic electrical relaxation rates for the Zr-Ta-mixed oxide $Li_{6.5}La_3Zr_{1.5}Ta_{0.5}O_{12}$. The rates are compared with hopping rates obtained from various NMR methods reported by our group and others (see [1]). Overall, Li^+ translational cation hopping processes are observed over a dynamic time window spanning seven decades

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Metals as Energy Carriers in a Future Hydrogen Economy

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A renewable, hydrogen-focussed energy system requires robust solutions for high-density energy storage and cost-effective large-scale transportation. Non-noble metals and metal oxides represent a promising pathway for accelerating hydrogen integration into sector-coupled energy systems by serving as solid energy carriers for a circular economy.

Among these materials, iron-based systems have emerged as particularly attractive candidates for energy storage, offering the capability to deliver both heat and high-purity hydrogen on demand. Chemical looping processes, operated at elevated temperatures, additionally provide intrinsic gas purification capabilities. In this approach, a hydrogen-rich gas stream acts as the reducing agent for the metal oxide. Subsequent oxidation with steam generates high-purity hydrogen, whereas oxidation with air is strongly exothermic, producing heat for energy applications. The practical deployment of such systems depends critically on the mechanical stability of the oxygen carrier materials, increased resistance to agglomeration and sintering, mitigation of impurity accumulation, and overall techno-economic and environmental performance [1]. To address these challenges, reactive metal oxides such as hematite (Fe_2O_3) were combined with high-melting stabilizing oxides, for example yttria-stabilised zirconia (YSZ). This strategy resulted in enhanced cyclic stability over extended redox operation and revealed a distinctive self-cleaning behaviour under carbon deposition conditions induced by CO-containing feed gas streams from reformed biogas [2].

Internal collaborations

Collaborations with the Institute for Solid State Physics have provided deeper insights into microscopic effects via X-ray-based analytics, resulting in improvements to contact mass development. The SOMAPP Lab's resources are being widely employed for the current research effort. The intention is to intensify research into material analytics and degradation mechanisms.

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Engineering Dehaloperoxidases for Phenolic Pollutant Removal

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Dehaloperoxidase (DHP) is a heme protein discovered in the marine annelid *Amphitrite ornata* [1]. Apart from serving as a hemoglobin for oxygen transport [2], it also functions as a catalytic enzyme [1]. In the presence of haloaromatic compounds secreted by species occupying the same ecological niche, it switches to a detoxifying peroxidase [1, 3, 4]. DHP exhibits activity towards halogenated and non-halogenated phenols and related aromatic compounds [5]. This makes DHP an attractive biocatalyst for the degradation of persistent organic pollutants widely used in industry.

We identified DHP homologs in related organisms showing a similar dual activity and provide an efficient *E. coli*-based expression system for the production of up to 100 mg/L of recombinant enzyme. Spectrophotometric assays and HPLC/MS showed that these enzymes are functional DHPs, exhibiting peroxidase and peroxygenase activity. To expand substrate specificity for efficient defluorination of fluorinated phenols, we use an enzyme evolution strategy supported by machine learning. To this end, we developed a medium-throughput screening of a combinatorial enzyme library for use in Bayesian optimization-guided machine learning combined with predictive computational methods.

Our findings indicate that DHP activity is much more widespread in nature than previously recognized, providing a new sequence space for enzyme engineering and enzymatic bioremediation.

Envisaged internal collaborations

Prof. Robert Peharz (Institute of Machine Learning and Neural Computation): Bayesian optimization-guided machine learning, computational prediction.

Prof. Torsten Mayr (Institute of Analytical Chemistry and Food Chemistry): Optical sensor for real-time H_2O_2 monitoring.

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Automated Construction and Property Exploration of Coordination Cages

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Building upon previous work with automated discovery, construction and optimisation of coordination cages,[1-5] this poster presents a new automated workflow for constructing and assessing coordination cages from topological blueprints and molecular building units.[6] Nitrogen-containing linker geometries are translated into an internal coordinate representation, combined with predefined cage topologies, and aligned through matrix-based placement to generate three-dimensional cage structures. The resulting models provide reproducible starting points for force-field pre-optimisation and semiempirical tight-binding refinement, enabling rapid structural assessment and comparison of candidate assemblies. As a demonstration, a literature photoswitchable cage was reconstructed in open- and closed-linker forms and examined through simulated UV–Vis spectra. The workflow supports efficient computational exploration of the coordination cage design space.

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Electrified Biocatalysis: Enzyme-Based Bioelectrochemical Systems for Value-Added Products

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A GMC (glucose–methanol–choline) family oxidoreductase from *Rhizobium* sp. GIN611 (*Rh*G3DH) encoded within a single glycoside utilization locus (GUL), is a FAD-dependent dehydrogenase that catalyzes C3 oxidation of various carbohydrates [1]. Structurally, *Rh*G3DH contains a 3Fe–4S cluster and forms a complex with a twin-arginine translocation (TAT) protein. *Rh*G3DH transfers electrons naturally to cytochrome c (CytC), while also displaying activity toward artificial inorganic redox mediators such as potassium ferricyanide ($K_3[Fe(CN)_6]$) [2]. In addition, *Rh*G3DH exhibits a broad substrate spectrum toward sugars and glycosides, tolerating diverse aglycones as well as *O*- and *C*-glycosidic linkages, independent of linkage position and α/β-configuration. Despite this broad substrate scope, the enzyme exhibited strict C3 site-selectivity at the non-reducing glycosyl residue and prevented overoxidation even at high conversion.

The electron-transfer capability of *Rh*G3DH toward $K_3[Fe(CN)_6]$ and CytC enables the construction of a mediated electron transfer (MET)- and direct electron transfer (DET)-type bioelectrocatalytic systems for carbohydrate oxidation, respectively. In these systems, electrons generated during *Rh*G3DH-catalyzed substrate oxidation are transferred to the electrode surface either via diffusional mediators or through CytC. MET-type systems often exhibit efficient and robust electron transfer owing to the presence of redox mediators with rapid electron-transfer kinetics and suitable redox potentials, thereby providing an effective driving force for enzyme regeneration. In contrast, DET-type bioelectrocatalysis eliminates the need for the small-molecule mediators [3]. Therefore, *Rh*G3DH provides a promising platform for saccharide/glycoside sensing [4] or an anodic biocatalysis in biofuel-cell-type devices [5].

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Envisaged internal collaborations

Collaborations with research groups specializing in enzyme-solid surface interaction analysis and material surface chemistry could be of potential interest.

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Design and Synthesis of N-Functionalized Derivatives of 2,5-Dideoxy-2,5-imino-D-mannitol (DMDP) as Selective Glycosidase Inhibitors

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Glycosidases are enzymes that catalyse the hydrolysis of glycosidic bonds and play central roles in numerous biological processes. Genetic mutations or post-translational defects can lead to severe pathological conditions, including diabetes, cancer and lysosomal storage disorders (LSDs). In this context, carbohydrate-based glycosidase inhibitors, such as DMDP (**A**), have been extensively described by our group as well as in general literature.[1-4]

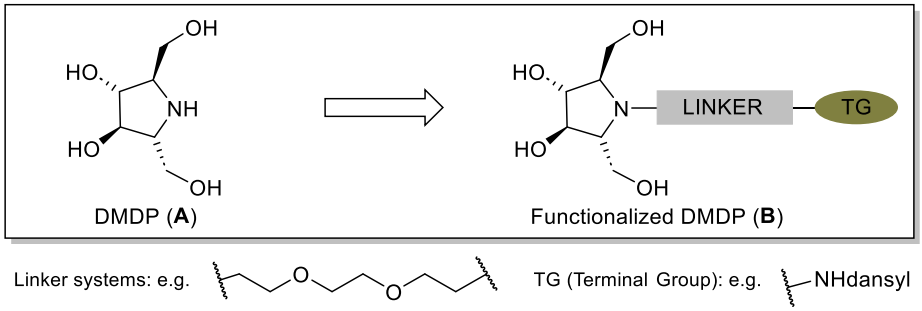

Figure 3: Examples of N-functionalized derivatives of DMDP

The aim of this project is the design, synthesis and biological evaluation of selective and powerful glycosidase inhibitors based on DMDP (**A**, 2,5-Dihydroxymethyl 3,4-dihydroxypyrrolidine). Strategic structural modifications by N-functionalization in the parent scaffold (**A**), enable structure–activity relationship studies aimed at improving potency and selectivity for specific glycosidase targets such as α- and β-glucosidases. Results and synthetic details will be presented.

Envisaged internal collaborations

For in-depth structural characterization, advanced NMR spectra are measured by Hansjörg Weber from the Institute of Organic Chemistry (TCVB). Crystallographic measurements are performed by Roland C. Fischer from the Institute of Inorganic Chemistry (TCVB).

Financial support: Austrian Research Foundation FWF, Weave Austria - Prague PIN 5558524 and the Czech Science Foundation (25 – 18949L) and WTZ (OeAD: MULT 01/2025 and Cz: 8x25048).

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Virtues and Merits of Pods in Discrete Element Method-based Simulations

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The modelling of real-world granular and soft matter systems is frequently constrained by traditional Discrete Element Method (DEM) approaches. These rely on idealized spherical particles that fail to capture the complex interlocking and non-convex behavior inherent in materials like battery recyclate, biomass, or polymer networks. This work introduces "pods": abstracted particle geometries such as dipods, tripods, and tetrapods formed by rigidly connected spheres, presenting a robust alternative for phenomenological modelling [1,2].

A first virtue of the pod framework is its governing dimensionless interlocking parameter (ξ/D). This parameter serves as a critical metric for the transition between free-flowing and interlocking behavior, acting as a "control switch" for the systematic investigation of shape effects on stacking, arching, and macroscopic material response. The aspect ratio directly introduces "geometric cohesion" while retaining the straightforward contact laws and overlap calculation of spheres. Computational cost remains low relative to alternative non-spherical representations such as polyhedra.

A further virtue is the framework's explicit treatment of simulation uncertainty. Pods introduce a Sensitive Dependence on Initial Conditions (SDIC), where infinitesimal variations in initial configurations are amplified by nonlinear contact interactions. By correlating pod complexity with this inherent variability, the framework provides rational guidelines for sample size determination, ensuring sufficient simulation repetitions to robustly capture chaotic outcomes in non-convex systems [3].

We further introduce *flexible pods*. In this extension, constituent arms contract toward the center of mass under load. This enables the simulation of highly compactable materials such as fibrous polymer recyclate. Arm contraction causes the constituent spheres to overlap. As a result, standard multisphere DEM no longer conserves particle volume or yields a consistent moment of inertia. To resolve it, we derive, implement, and validate a Constant Volume (CV) correction model for multisphere bodies in LIGGGHTS-PUBLIC 3.8.0. Exact closed-form expressions for overlap volume and moment of inertia are obtained as functions of the deformation parameter $x = \xi/D_0$. A unified degree-5 polynomial fit, generalised across dipod, tripod, and tetrapod geometries, replaces per-timestep numerical integration. Volume errors stay below 0.32%, benchmarked against Monte Carlo integration with 12 million samples.

We demonstrate the framework on two applications. First, we model hydrogels as networks of tetrapods connected by a harmonic potential. Second, we use flexible pods to simulate compaction of fibrous materials. Alongside these, we provide concrete guidelines for sample size determination in chaotic non-convex systems, derived from the SDIC analysis. Together, these results establish pods as a tractable route to predictive simulation of complex, non-convex, and deformable particle systems at industrial scale.

Envisaged internal collaborations

The pod framework is built on simulation, yet its predictive power ultimately rests on comparison with physical measurements. A collaboration track centred on experimental validation of interlocking and packing behaviour is envisaged with groups in the TCVB Faculty.

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Synthesis of Glycoamphiphilic Structures for the Assembly of Glyco-Nanodiscs [1]

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Nanodiscs are used to extract and stabilize membrane proteins from cellular membranes while retaining their native environment by incorporating a nanoscale lipid bilayer. Membrane-scaffold-protein (MSP)-based nanodiscs require detergent extraction of the protein and reconstitution into an artificial lipid bilayer. Polymer- and **carbohydrate-based nanodiscs** directly extract the protein, including its immediate lipid environment, from the **natural** membrane.[1-3]

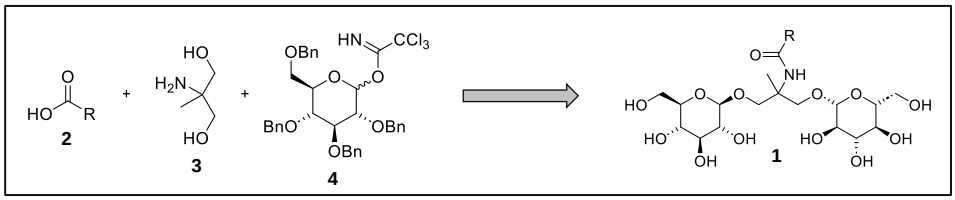

Fig.1: General synthesis scheme

Synthetic approach: We have developed a concise and modular synthetic approach allowing for straightforward variations of all components present in the glycoamphiphiles. Fatty-acid **2** was coupled to amino-diol **3** via the "mixed-anhydride method". Subsequently, *O*-(2,3,4,6-tetra-*O*-benzyl-D-glucopyranosyl)-trichloroacetimidate (**4**) was employed in a Schmidt glycosylation to obtain target compound **1** upon deprotection.[4-5] Previously, instead of fatty-acid **2**, its corresponding acid-chloride had been utilized. Due to limited commercial availability of various acid chlorides, an alternative procedure was necessary to form the amide directly from carboxylic acids. Experimental details and results will be presented.

Envisaged internal collaborations:

For in-depth structural characterization, advanced NMR spectra are measured by Hansjörg Weber from the Institute of Organic Chemistry (TCVB). Crystallographic measurements are performed by Roland C. Fischer from the Institute of Inorganic Chemistry (TCVB).

Financial support: Austrian Research Foundation FWF, Weave Austria - Prague PIN 5558524 and the Czech Science Foundation (25 – 18949L) and WTZ (OeAD: MULT 01/2025 and Cz: 8x25048).

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In-line monitoring of oxygen, pH, glucose and lactate in organ-on-chips with integrated optical sensors

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c) Department for Microphysiological Systems, Institute of Biomedical Engineering, Faculty of Medicine, Eberhard Karls University Tübingen, Tübingen, Germany

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Constant monitoring of culture parameters like oxygen, pH, and glucose is needed to ensure physiological conditions in micro physiological systems, such as Organ-on-a-Chips (OoC). Furthermore, the measurement of these parameters can give valuable information on the viability and metabolic state of the cultured cells. Despite the large improvement of organ-on-chip systems in the recent years there is a lack in the development of efficient in-situ readout techniques for micro physiological systems and organ-on-chips. Especially, metabolic monitoring is crucial to understand the cells response to different stimuli, e.g. by new pharmaceutical substances.

Analysis of organ-on-chips is challenging due to the small dimensions and sample volumes. Currently, this is mainly achieved by optical and fluorescence microscopy using stains and labels, which can be used for one single measurement. In recent years our group has established integration of sensors for the key metabolic and culture condition parameters oxygen, pH, glucose and lactate. Miniaturized luminescent sensors spots are integrated into various microfluidic cell and tissue culture devices using inkjet printing technique. The sensor spots in a size from 300 to 800 µm. All sensors can be read-out with the same optical platform, which based on commercially available miniaturized phase fluorimeters.

We present microfluidic cell chips with integrated sensors and performance data. We demonstrate monitoring of the metabolism in organ-on-chips applying mitochondrial stress tests and model drugs. These results enable the way for multi-parametric continuous assessment of cell metabolism in complex microfluidic systems. The sensor technology is versatile and can easily transferred to other organ-on-chip devices and paves the way for multi-parametric continuous assessment of metabolism for standardized drug screening.

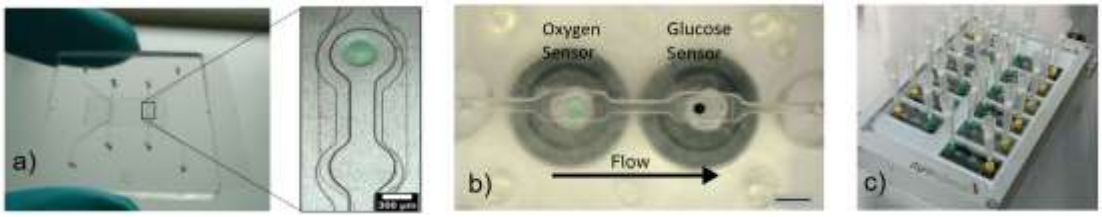

Figure 1. a) Heart-on-Chip with integrated optical oxygen sensors (green dots) [1] b) Sensor integrated in a microfluidic flow cell c) Ensemble of microfluidic chip with sensor read-out system

Envisaged internal collaborations

We offer collaborations in any field were the application and research on luminescent sensors is beneficial and sought.

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Mechanically Tunable 3D-Printed Hydrogels via Dual Enzymatic and Ionic Crosslinking

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The integration of biopolymers into 3D printing, particularly polysaccharide-based hydrogels, has substantially advanced tissue engineering and regenerative medicine. In this study, we report the development and characterization of 3D-printed biomaterials based on alginate modified with tyramine (Alg-TA), combined with nanofibrillated cellulose (NFC), glucose, calcium carbonate ($CaCO_3$), and the enzymatic system glucose oxidase (GOx) and horseradish peroxidase (HRP). A dual-enzyme crosslinking strategy enables solution-free gelation through synergistic ionic and covalent mechanisms: in situ generation of H_2O_2 drives HRP-mediated covalent crosslinking, while $CaCO_3$ facilitates simultaneous ionic crosslinking.

The resulting scaffolds exhibit a tensile strength of 0.13 ± 0.02 N/mm² and an elongation at break of 77 ± 4%, whereas formulations without $CaCO_3$ display higher tensile strength (0.26 ± 0.04 N/mm²) but reduced elasticity (36 ± 3%). The constructs demonstrate excellent print fidelity, mechanical integrity, and dimensional stability. Systematic evaluation of crosslinking parameters, including pH, glucose and enzyme concentrations, and atmospheric conditions, reveals a complex interplay governing scaffold formation and performance. Overall, the developed bioink platform offers a versatile and promising approach for fabricating mechanically robust, adaptable, and biocompatible scaffolds for regenerative medicine applications.

Envisaged internal collaborations

We envision collaborations with TCVB groups in biomaterials, tissue engineering, and biofabrication to optimize the printability and performance of our dual-crosslinked Alg-TA/NFC scaffolds. Partnerships with cell biology and regenerative medicine experts will support evaluation of cell adhesion, proliferation, and matrix remodeling.

Cooperation with groups in rheology, soft matter mechanics, and structure–property analysis will help clarify how formulation and process parameters affect scaffold formation and mechanical behavior.

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Entropy Measurements to Investigate Hard Carbon as a Battery Active Material

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Hard carbon is a promising material for the use as an anode in sodium-ion batteries, a rising technology that aims to replace the resource-hungry lithium-ion battery, especially in stationary applications. It is, however, unclear how sodium ions are stored in the material due to its disordered nature [1]. Entropymetry is a method that has not yet been applied for the in-situ characterization of hard carbon, investigating the storage mechanisms of ions in an electrode based on their effect on the entropy of the material [2]. Evaluation of the entropy change across the entire capacity of a set of hard carbon half cells shows a progression that depicts multiple regions. Additionally, the shape of the progression may indicate that certain storage locations are not completely filled after sodiation of the hard carbon, suggesting that it could be possible to further increase the capacity in these cells.

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Support-Assisted 3D Printing of Cellulose Hydrogels for Complex Biomimetic Architectures

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Three-dimensional (3D) printing of hydrogels has enabled new directions in biomedical engineering, soft material design, and biofabrication. However, unsupported hydrogel inks often collapse under their own weight or deform during printing, limiting achievable geometries.[1,2] We present a reproducible, standardized support system combining a nanofibrillated cellulose/sodium alginate (NFC/ALG) structural ink with a cellulose-based sacrificial support ink composed of NFC, hydroxyethylcellulose (HEC) and $CaCl_2$, building on established NFC-based hydrogel systems and support-assisted printing concepts, shown in Figure 1.[3,4] Quantitative validation using tubular models shows that unsupported tubes collapse before 50 mm height, whereas supported tubes remain upright and stable. Surface fidelity is substantially improved by reducing layer height, yielding watertight prints. Demonstrations of complex geometries, including an anatomical aorta, confirm the method's capability. Support dissolution in 30 mM $CaCl_2$ occurs over approximately 3 days, ensuring stability during crosslinking and handling. Compared with other sacrificial strategies, this approach is inexpensive, cellulose-based, and relies on mild ionic crosslinking compatible with future cell-laden systems. This work provides a robust and accessible hydrogel engineering system, supporting stable and high-fidelity DIW of complex anisotropic structures.

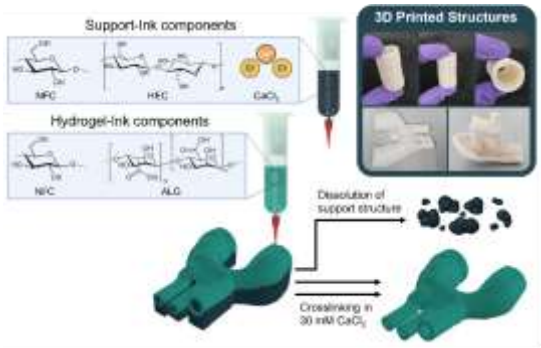

Figure 1: Cellulose-based sacrificial support enables stable printing of complex hydrogel

Possible internal collaborations

Possible joint projects with the Institute of Process and Particle Engineering and the Institute of Molecular Biotechnology by combining the printed hydrogel constructs with immobilized living cells. The sacrificial support printing strategy could further enable the fabrication of fine perfusable flow channels for advanced hydrogel-based continuous flow bioreactors and engineered living materials.

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Material Properties Shaping Performance and Stability in Organic and Perovskite Solar Cells and Organic Field-Effect Transistors

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The performance and operational stability of emerging solar cells and organic field-effect transistors are influenced not only by the chemical design and intrinsic properties of the active materials, but also by their processing conditions, morphology, and interfaces. This poster highlights examples how targeted material development and advanced characterization can reveal and control these relationships in organic solar cells, perovskite solar cells, and organic field-effect transistors.

For organic solar cells, we show that both active layer morphology and interfacial engineering are decisive for device performance and photostability. In PM6:Y6 bulk heterojunction solar cells, the commonly observed initial burn-in loss can be strongly suppressed by combining PEDOT:PSS with the self-assembling molecule 2PACz as a bilayer hole transport layer. Transient photovoltage measurements indicate that this improved stability is related to less interfacial disorder induced through photo-aging. In a further study, a detailed STEM/EELS analysis of D18:L8-BO blends reveals how donor network formation and donor dilution influence charge generation, charge collection, and optical properties, providing design guidelines for efficient semitransparent organic solar cells.[1]

In perovskite photovoltaics, we address strategies to improve both lead-based and lead-free absorber systems. For quasi-2D perovskites, conjugated diammonium spacers and additives improve crystallographic orientation, reduce defect densities, and enhance device efficiency and stability.[2] For tin halide perovskites, tailored composition, interface engineering, and optimized antisolvent processing contribute to efficiencies above 14% and operational stability exceeding 1000 h under maximum-power-point conditions.

Moreover, in the field of organic field-effect transistors, a study on the sustainable synthesis and processing of BTBT-based semiconductors demonstrates how molecular side-chain design influences film formation and field-effect mobility. Overall, these studies show how targeted control of materials, interfaces, and processing can enable more efficient and stable solar cells and transistors.

Envisaged internal collaborations

Collaborations are ongoing with the Institute of Inorganic Chemistry for GIWAXS and AFM measurements, and with the Institute of Analytical Chemistry and Food Chemistry for PL characterization of organic and perovskite thin films.

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Synthesis of ApoA1 Mimetics

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Apolipoprotein A1 (ApoA1) is a crucial member of the blood apolipoproteins and serves as a major component of high-density lipoprotein (HDL). ApoA1 has substantial potential as a carrier for small interfering RNA (siRNA) into tumor cells expressing scavenger receptor B1 (SR-B1). Evidence supporting the beneficial effects of ApoA1 in reducing atherosclerosis has been demonstrated through studies where mice were treated with purified ApoA1 and in mice with transgenic or adenoviral-mediated overexpression of the human ApoA1 gene.[1] Considering the anti-inflammatory properties and immune regulatory functions of ApoA1, it is evident that this apolipoprotein has significant potential as an anti-tumorigenic agent.[2] ApoA1 exhibits 90 % amphipathic α-helical content.[2] Helical surface mimetics use conformationally restricted scaffolds with attached functional groups that mimic the i+1, i+2, i+2 and i+5 pattern of side-chain positioning of an α-helix (Figure 1).[3]

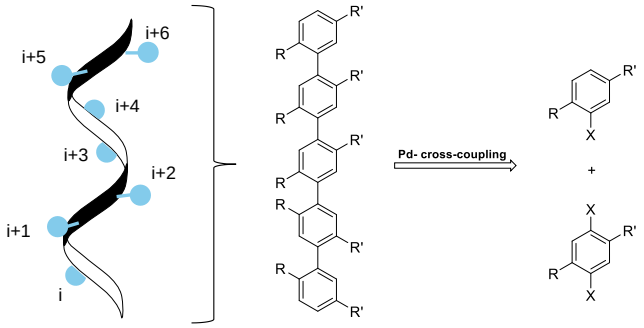

Figure 4: Assembly of pentaryl-based alpha-helix mimetics (R = lipophilic, R‘ = hydrophilic, X = BPin, I).

Previous research on ApoA1 mimetics, which are based on small amphipathic peptides, has demonstrated promising results. However, these mimetics face challenges related to selectivity and stability.[4] Consequently, our group investigated the synthesis of an amphipathic pentaryl ApoA1 mimetic to address these issues. The α-helical structure should be imitated using pentaryls with both hydrophilic and lipophilic side chains (Figure 1). The design is inspired by the structure of ApoA1 and existing peptide-based ApoA1 mimetics.

Envisaged internal collaborations

None

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Machine Learning-Driven Process Engineering and Manufacturing

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Machine learning and AI-based approaches are used today in many different areas of process engineering. To illustrate that diversity, this paper presents project examples from two different domains.

Machine Learning-Driven Roll-to-Roll Manufacturing for thin-film materials: The scalable production of thin-film materials, such as membrane electrode assemblies (MEAs) for fuel cells and electrolysers, is limited by complex process interactions and insufficient in-line quality control [1]. We are developing a novel roll-to-roll manufacturing platform combined with machine learning (ML) for continuous, data-driven production. By integrating in-line sensor data with ML models, key process steps such as material coating and drying can be monitored and optimized in real time. The approach improves coating uniformity, material utilization, and electrochemical performance while reducing experimental trial-and-error. Building on recent advances in ML-assisted optimization [2], this framework transfers data-driven process control from laboratory-scale studies to scalable industrial manufacturing. The work is strengthened through the joint “Coat&Roll” initiative with the **ICTM, IBioSys and BPTI** institutes of the TCVB Faculty, enabling future collaborative research projects based on shared roll-to-roll infrastructure.

Figure 1: Roll-to-Roll Coater (Sample image: FOM moduloR2R)

Machine Learning-Augmented Integral Equation Theory for Materials Design: Accurate predictions of liquid structure and thermodynamic properties are crucial for the development of advanced materials, electrolytes, and catalytic systems. To enable such predictions based on molecular properties, statistical physics is combined with machine learning by training a deep operator network on molecular simulation data to complement an integral equation-based model [3]. The model is trained on correlation functions extracted from Monte Carlo simulations across a wide range of temperatures and densities and yields a closed system of equations within the Ornstein-Zernike framework. In collaboration with the Elettra-Sincrotrone Trieste group at the **AC** institute of the TCVB Faculty, the calculated results of the model will be validated against experimental static structure factors from synchrotron scattering measurements, establishing a direct link between data-driven simulations and real material systems.

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Spatially Tunable Photopolymer Networks

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Using light to control both the formation and the structural/mechanical properties of polymers represents one of the most powerful strategies in modern polymer science. In this context, dynamic covalent exchange reactions provide unique opportunities to introduce stress relaxation, self-healing, and reprocessability into photopolymer materials. [1] In our work, dynamic properties can be activated locally and on demand by varying the wavelength of light during curing and activation of exchange reactions. By incorporating photoacid generators (PAGs) [2] and photobase generators (PBGs) [3] as latent transesterification catalysts, Brønsted acids or bases are generated locally upon UV exposure and efficiently catalyze thermo-activated transesterification reactions. Combined with chemical amplification concepts [4], this enables enhanced control over exchange reaction kinetics and network adaptability. Furthermore, a catalyst-free strategy based on disulfide exchange reactions was explored, where wavelength-selective curing enables the formation of either dynamic disulfide-containing networks with pronounced stress relaxation or predominantly static photopolymers with suppressed relaxation behavior. [5]

These concepts significantly expand the design freedom of photopolymer-based additive manufacturing and establish a versatile platform for multifunctional materials with spatially programmable properties. In the future, such light-controlled CAN systems are expected to play an important role in biomedical and pharmaceutical applications, including tissue-mimetic scaffolds, adaptive implants, responsive drug delivery systems, and smart medical devices.

Envisaged internal collaborations

This research was performed in collaboration with Dr Max Schmallegger (Institute of Physical and Theoretical Chemistry). Future work is planned in collaboration with Prof Eva Roblegg (Institute of Pharmaceutical Science at the University of Graz) to establish these materials for biomedical and pharmaceutical applications, while a collaboration with Prof Michael Haas (Institute of Inorganic Chemistry) would further enable the exploration of novel photoinitiators for advanced light-controlled material systems.

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Programming Cellulose Assembly and Morphology through Enzymatic Control of Chain Polymerization

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Cellodextrin phosphorylases (CdPs) enable controlled synthesis of short-chain cellulose, but how differences in enzyme behavior influence cellulose structure and morphology remains unclear.[1] Here, we show that CdPs regulate not only cellulose chain elongation, but also the assembly pathway of the resulting materials. By comparing diverse CdPs, we identify enzyme-dependent polymerization behaviors ranging from short, narrowly distributed cello-oligomers to chains beyond DP 20 with broader distributions. These differences arise from the combined effects of substrate-binding pocket architecture and enzyme activity, which regulate sustained elongation, productive chain rebinding, and aggregation in solution.

This molecular control is reflected in the resulting cellulose material morphologies. Narrow chain-length distributions favor cellulose II-like organization and sheet-like micrometer-scale assemblies. In contrast, reaction conditions that enable sustained chain elongation and broader chain-length distributions give rise to cellulose IV_{II}-like diffraction features and spontaneous assembly into micrometer-scale beads. Together, these findings connect CdP-controlled chain growth with cellulose crystallinity and morphology, providing a basis for enzymatic design of cellulose materials from the molecular level upward.

Envisaged internal collaborations

Collaboration with research groups at institutes of biochemistry, inorganic chemistry, physical chemistry, organic chemistry, and environmental biotechnology such as Glen Smales for SAXS investigations, Max Schmallegger for XRD investigations, Hansjörg Weber for NMR investigations, and Angelika Battisti for optical microscopy measurements.

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Illuminating reaction mechanisms: spectroscopy-led insights from photoinitiated polymerization to photoresponsive materials

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Our group operates at the interface of physical chemistry, photochemistry, and radical chemistry to resolve how radicals, radical ions, and photoexcited states control reactivity in polymerization, catalysis, and functional materials. A central focus is photoinitiated radical polymerization: we benchmark photoinitiators, particularly Ge/P-based systems, for advanced polymers and polymer-based materials[1], quantify primary radical formation and termination pathways[2], and use light to tailor polymer microstructure. Beyond photopolymers, we investigate antioxidants and oxidative stress, radical processes in biomimetic membranes[3], photocatalysis,[4] photoresponsive materials, and light-driven molecular switches.[5]

Our toolkit integrates time-resolved electron paramagnetic resonance (EPR), nuclear magnetic resonance (NMR) and chemically induced dynamic nuclear polarization (CIDNP) spectroscopy, (time-resolved) optical spectroscopy and laser-flash photolysis (LFP), cyclic voltammetry, kinetic modelling and computational chemistry to identify transient intermediates, evaluate reaction channels and extract rate constants and spin dynamics.

Envisaged internal collaborations:

We invite projects where mechanistic, spectroscopy-anchored insight can accelerate discovery. We offer:

- Characterization of light-active molecules and materials
- Mechanistic insights into radicals and photoexcited states
- On-demand spectroscopy/characterization: time-resolved EPR, CIDNP, LFP, UV-Vis and XRD
- Photophysical/electrochemical profiling: redox windows, lifetimes, wavelength dependence
- Kinetic modelling and computational support (DFT)

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Marker-Free Co-Production of Industrial Enzymes and Natural Pigments in *Komagataella phaffii*

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c) Institute of Molecular Biotechnology, Graz University of Technology, NAWI Graz, Graz, 8010, Austria

Microbial co-production of multiple value-added products within a single fermentation represents a powerful strategy to enhance the economic and environmental sustainability of bioprocesses. Here, we report the first experimental demonstration of marker-free co-production of a secreted industrial enzyme and an intracellular natural pigment in *Komagataella phaffii*. Using the beetroot (*Beta vulgaris*) pigment betanin as a model metabolite and *Candida antarctica* lipase B (CalB) as a model enzyme, we engineered strains capable of simultaneous pigment biosynthesis and efficient protein secretion. To enable food- and feed-compatible production, we developed a pMAPS-based marker-free genomic integration system, yielding stable, antibiotic-free strains with integration efficiencies of up to 1.8%. This system simplifies regulatory compliance and enables rapid phenotypic screening of multi-gene pathway integrations. Notably, this work constitutes the first report of betanin biosynthesis in *K. phaffii*. Using a strong derepressible promoter, CalB secretion was evaluated before and after methanol-induced betanin production. We demonstrate that (i) betanin was efficiently excreted into the culture supernatant; (ii) betanin co-production had little to no impact on CalB secretion in shake-flask and bioreactor cultures; and (iii) CalB could be efficiently purified from pigment-containing supernatants. Collectively, these results establish *K. phaffii* as a robust chassis for the dual production of enzymes and high-value metabolites, enabling valorization of fermentation biomass and broth that would otherwise be discarded. This strategy is immediately applicable to natural pigments such as betanin and is readily extensible to other metabolite classes, providing a versatile platform for sustainable and economically viable microbial manufacturing.

Envisaged internal collaborations

Andreas Winkler, Assoc.Prof. Dipl.-Ing. Dr.techn., Barbara Siegmund, Assoc.Prof. Dipl.-Ing. Dr.techn., Erich Leitner, Univ.-Prof. Dipl.-Ing. Dr.techn., Gustav Oberdorfer, Ass.Prof. Priv.-Doz. Mag.rer.nat. Dr.rer.nat., Regina Kratzer, Assoc.Prof. Dipl.-Ing. Dr.techn., Rupert Kargl, Assoc.Prof. Mag.rer.nat. Dr.rer.nat., Susanne Lux, Assoc.Prof. Dipl.-Ing. Dr.techn.

Flavour Chemistry and Sensory Science to Address Current Challenges in Fruit Cultivation

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Fruit and vegetable cultivation has a long-standing tradition in European countries and constitutes a key pillar in ensuring food security. However, globalisation, climate-change and changing consumers' demands pose new challenges for agriculture. Consumers demand fruits with pronounced flavour and long shelf-life, preferably organically grown and produced without long-distance transportation. Climate change alters site conditions leading to elevated average temperatures, changed precipitation cycles, late winter onsets and the emergence of new pests (i.e. insects and/or fungi) in the orchards. Contamination by microorganisms that thrive under the altered conditions in the soil, water or on the fruit surface can lead to the development of pronounced off-flavour in the agricultural crops resulting in significant economic losses [1].

Many fruit cultivars (e.g. Golden Delicious apples) which have been cultivated for decades no longer meet these requirements. New cultivars with a crisp texture, extended storage capacity, pronounced flavour and resistance to fungal diseases may replace those cultivated since the 1970s [2,3]. However, for perennial plants, changing a cultivar requires several years before achieving full yield. Therefore, careful investigation is necessary beforehand to avoid misinvestment by fruit growers.

In this contribution, we demonstrate how flavour chemistry and sensory science contribute to a deep understanding of the biochemical processes in the fruits, from growth and on-tree maturation to the processes taking place during postharvest ripening. Particularly for climacteric fruits, which show ripening processes even after the harvest, an in-depth understanding of the biochemical reactions that ultimately lead to flavour formation is essential. Identification of volatile and potentially odour-active compounds using mainly gas chromatographic techniques gives insight into the biochemical reactions in the fruit during development. This also allows to draw conclusions about the up- and down-regulation of enzyme activities under altered conditions. Sensory evaluation allows insight into the associated sensory changes of crop.

Envisaged internal collaborations

- Institute of Environmental Biotechnology, TU Graz, **Birgit Wassermann** ass. Prof., **Wisnu Wicaksono**, PhD to investigate the impact of the plant microbiome on the formation of the flavour of fruits.
- Institute of Molecular Biotechnology, TU Graz, **Harald Pichler**, assoc. Prof. to achieve a deeper understanding of climate-change induced up- and downregulation of enzymes involved in bioflavour flavour formation.

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Harnessing carbenoid reactivity from imidazoles and oxiranes

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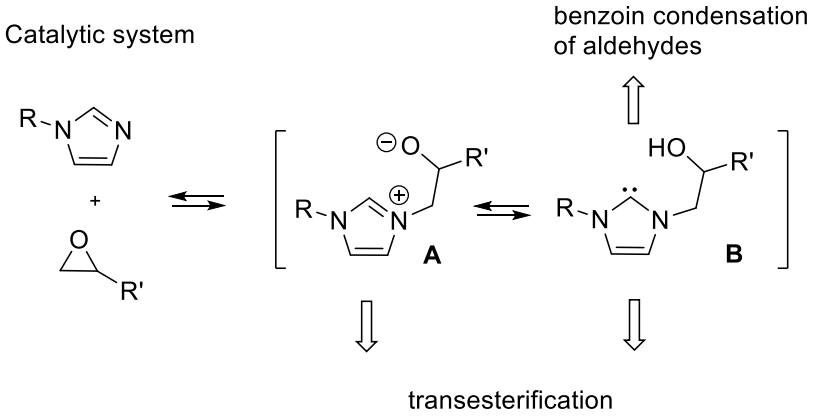
The combination of azole compounds, such as 1-methylimidazole and oxiranes gives carbenoid reactivity at elevated temperatures. Benzoin condensation was performed with 5 mol% azole and 10 mol% oxirane under air at temperatures of 70°C and above, achieving conversions of up to 85% of benzaldehyde and yields of up to 64% of benzoin. The lower benzoin yield is due to the formation of oxidative benzoin follow-up products under these reaction conditions. Thus, a modular, potentially inexpensive method of generating carbenoid reactivity has been revealed [1].



The practical utility of this catalytic system was demonstrated by polymerizing simple bifunctional aldehyde/oxirane monomers, such as the renewable vanillin-based 2-methoxy-4-(2-oxiranylmethoxy)-benzaldehyde—using 5 mol% 1-methylimidazole in a solventless manner and without excluding air. The monomers polymerized via both the formyl and the oxirane groups, yielded thermosets with glass transition temperatures above 100°C [1]. Application of the catalytic system in poly(ethylene terephthalate) glycolysis and in the ring opening polymerization ε-caprolactone is also discussed [2].

Envisaged internal collaborations

We are studying organocatalytic transformations, particularly polymerization and depolymerization reactions, and are eager to test our catalysts in your reactions.

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Application of 1,5-Dideoxy-1,5-L-iditol (DIJ) Presenting Ligand Directed Chemistry Probes for Labeling of Different Glycoside Hydrolases

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The ligand-directed chemistry (LDC) approach allows site-selective protein labeling of enzymes through proximity-driven covalent modification of amino acids located near the active site. [1] By using a reversible inhibitor as ligand for protein recognition, the intrinsic activity of the enzyme is restored after the labeling process. Based on our developed synthetic building block concept, different ligands, electrophilic reactive groups, linker moieties and terminal tags can be introduced. [2-4] Employing various different imino- and isoiminosugars as ligand, a comprehensive collection of ligand-directed chemistry probes was synthesized, targeting respective glycoside hydrolases. Biological evaluation of the invented LDC probes give insights into inhibition profile and labeling properties. Promising candidates are analysed towards their labeling efficiency by intact protein mass spectrometry. This study focuses on the results of probes incorporating the iminosugar 1,5-dideoxy-1,5-L-iditol as ligand, allowing for chemical modification of a specific target glycoside hydrolases including the identification of the labeling site from beta-glucosidase from *Thermotoga maritima* (GH1). Synthetic details and results from the biological evaluation of synthesised compounds will be given.

Envisaged internal collaborations

For in-depth structural characterization, advanced NMR spectra are measured by Hansjörg Weber from the Institute of Organic Chemistry. Intact protein mass spectrometry is performed by Andreas Winkler and Philipp Pelzmann from the Institute of Biochemistry and crystallographic measurements are performed by Roland C. Fischer from the Institute of Inorganic Chemistry. Concerning enzyme kinetics, we have a collaboration with Bernd Nidetzky from the Institute of Biotechnology and Biochemical Engineering. Protein expression has been conducted in collaboration with Margit Winkler, formerly at the Institute of Biotechnology.

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Materials Design and Sustainable Synthesis for Organic Electronics

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The sustainability of electronic materials and their processing is becoming increasingly important for the development of future device technologies. Within the GreenOMorph project, TU Graz contributes to this effort through the design, synthesis, and processing of functional organic materials while maintaining the performance and processability needed for electronic and sensing applications.

One area of research focuses on non-fluorinated, bio-derived piezoactive materials for printed ferroelectric sensors, where amino acids and peptides are investigated as sustainable molecular building blocks. Initial studies on alkyne-functionalized peptide systems have been carried out to enable further assembly and processing approaches.

In the field of small-molecule organic semiconductors, more sustainable synthetic methodologies are explored. P-type semiconductors based on thienoacene cores such as BTBT are prepared using greener solvent systems and alternative reaction conditions to obtain functionalized derivatives. In parallel, n-type semiconductors based on non-fused molecular architectures are investigated, where bulky side groups and non-covalent conformational locking motifs support molecular planarity and efficient π–π stacking. The influence of end-group modifications is additionally evaluated by DFT calculations.

Furthermore, sustainable synthetic strategies toward organic mixed ionic–electronic conductors for organic electrochemical transistors are evaluated, with particular emphasis on replacing hazardous reagents and solvents in benchmark polymer systems. Altogether, these activities illustrate a materials-focused contribution within GreenOMorph aimed at improving sustainability across different classes of organic electronic and sensing materials.

Envisaged internal collaborations

Internal collaborations include cooperation with the research group of Sergey Borisov for optical and advanced analytical characterization of functional organic materials. Potential future collaboration with the group of Michael Haas may support the synthesis and characterization of new materials relevant to organic electronics.

Harnessing Environmental Microbial Diversity for Human Health: Insights from Meta-Analysis and Fermented Food Systems

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Abstract
Environmental microbiomes represent a critical reservoir of functional diversity with direct relevance to human health, yet their contribution is often overlooked in current biotechnological frameworks. Through meta-analysis of microbiome datasets from healthy and disease cohorts, we show that reduced exposure to environmentally derived microbial diversity is consistently associated with altered community structure and functional imbalance in the human microbiome. Notably, disease-associated states are characterized by the depletion of low-abundant and environmentally linked taxa, indicating that these microorganisms may play key roles in maintaining system stability and immune regulation.

From an environmental biotechnology perspective, fermented food systems can be viewed as scalable and controllable platforms that bridge environmental and human microbiomes. These systems harbor complex microbial consortia originating from raw materials and processing environments, including phylogenetically diverse and rare taxa that are frequently lost in industrialized production. Such communities provide a unique opportunity to explore function-based microbial selection, metabolic interactions, and resilience mechanisms relevant for biotechnological applications.

Advances in meta-omics, microbial ecology, and systems biology now enable the identification and engineering of microbiomes, supporting the development of next-generation, community-based probiotic solutions. Integrating environmental microbial diversity into engineered systems offers new opportunities to restore functional balance in the human microbiome, particularly in the context of immune-mediated and autoimmune diseases. Overall, this work positions environmental microbiomes as a key resource for biotechnology, emphasizing the need to harness rare and functionally complementary taxa from food and environmental systems to develop sustainable, diversity-driven interventions for human health.

Potential internal collaborations
The joint project aims to advance the development of next-generation probiotics through strategic collaboration with the Institute of Biotechnology and Biochemical Engineering, focusing on scaling complex microbial consortia, optimizing fermentation processes, and enhancing the production of beneficial metabolites. This will support the development of stable, efficient, and industry-relevant probiotic systems. Partnership with the Institute of Molecular Biotechnology will enable genomics-driven identification of key microbial taxa and metabolic pathways, while metabolic modelling will guide the design of function-oriented microbial consortia. Collaboration with the Institute of Biochemistry will provide mechanistic insights and support functional validation of microbial interactions and metabolites. In addition, joint efforts on immobilization and delivery systems will enhance microbial stability, viability, and application potential, including the development of biocompatible matrices and advanced cultivation strategies. Overall, this integrated approach bridges environmental microbiology with scalable biotechnology, enabling the translation of microbial diversity into practical and sustainable health solutions.

Modular Synthesis of Teraryl-based Alpha-Helix Mimetics

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The inhibition of protein-protein-interactions (PPIs) with small molecules has become a new paradigm in Chemical Biology.[1] Hamilton and co-workers have shown that trisubstituted linear terphenyls can function as α-helix mimetics, displaying the i, i+4 and i+7 amino acid residues.[2] To address solubility issues, our group has developed a modified design, in which pyridine nitrogen atoms are introduced at the water-exposed face distal to the protein binding site. Most recently, we have achieved comprehensive coverage of the protein sequence space by assembling teraryls from a library of readily available building blocks decorated with the side chains of all proteinogenic amino acids relevant for PPIs (Fig. 1).[3,4,5]

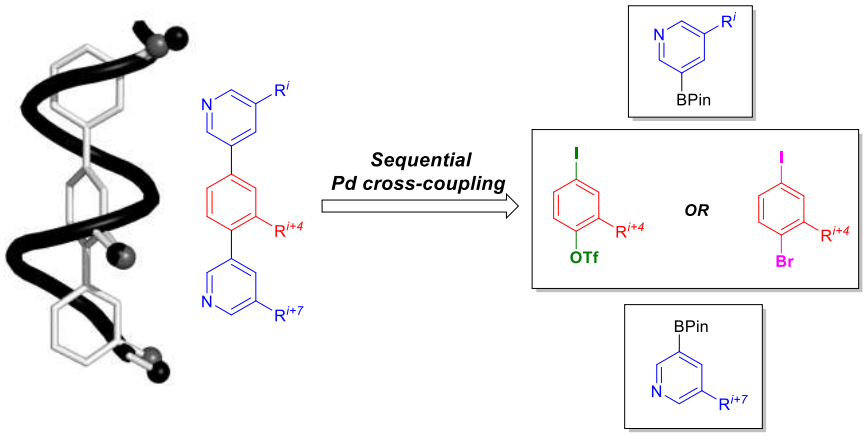

Figure 5. Assembly of teraryl-based alpha-helix mimetics.

Envisaged internal collaborations

None

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Molecular and Microbial Aspects in Biological Insect Control

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Productive and sustainably functioning agroecosystems are the basis for food security. Insects occur in agricultural systems as both pests and beneficial organisms. While some species occur as devastating pests, insects are also becoming industrially increasingly relevant as pollinators, as a protein source in the food industry or as decomposers of organic waste. Pest insects in agricultural systems can be controlled, among other things, by insect-pathogenic microorganisms. These so-called entomopathogens possess several molecular mechanisms that allow them to conquer the insect body by modulating or inhibiting the physiological and immunological defence mechanisms of their hosts. Chitinases, proteases, and lipases of entomopathogens can degrade the cuticle, the insect's outer protective layer. Once in the insect body, a variety of secondary metabolites can modulate or suppress the insect's immune response, while antibiotic secondary metabolites suppress the growth of other microbes within the insect's body. The identity, mode of action, and activity of these secondary metabolites, as well as entomopathogen interactions with the insect immune system and other microbiota colonizing the insect body are insufficiently understood. Therefore, research in this area holds immense potential for identifying novel bioactive metabolites, investigating the structure-activity relationship with respect to host range of entomopathogens, compatibility of entomopathogens with crop plants, optimizing insect pest biocontrol strategies, characterizing virulence marker genes, but also developing protection strategies against entomopathogens in beneficial insects. Therefore, this highly interdisciplinary research field has many thematic overlaps with other research areas within the TCVB Faculty.

Envisaged internal collaborations

Within the TCVB, our research has thematic overlaps with organic and analytic chemistry (secondary metabolite identification and measurement, compatible polymers for enhancing shelf life and entomopathogen formulation), biochemistry, molecular biotechnology (comparative structure biology of virulence-mediating enzymes, analysis of insect immune responses), and biochemical engineering (upscaling of entomopathogen production).

Metal-organic frameworks (MOFs) responsive colorimetric sensor for real-time monitoring of food quality

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Biogenic amines (BAs) are important indicators of food spoilage, produced when protein-rich foods such as meat, eggs, and dairy products deteriorate [1]. Monitoring their presence in real time is crucial for ensuring food safety. Traditional detection methods, however, are often complex, expensive, and unsuitable for on-site applications.

The FRESCO (Food Responsive Sensor for Colorimetric Observation) project addresses this challenge by integrating metal-organic frameworks (MOFs) into flexible packaging materials. MOFs are a class of porous crystalline materials that have emerged as promising platforms for colorimetric sensing because of their tunable structures and effective interactions with guest molecules [2]-[4].

In this project, porphyrin MOFs are used as responsive sensing materials. MOFs are deposited onto robust porous substrates and protected by polymer coatings. This process enables the fabrication of a MOF-based sensing device. The interrogation of the sensor was inspired by reported food spoilage sensing platforms [5]: the MOF sensor is incorporated into a portable platform that allows users a straightforward readout of the color change. Upon exposure to volatile biogenic amines, the MOF sensors exhibit rapid and visible color changes, providing a real-time monitoring of food freshness.

By providing a simple visual response to food freshness, this affordable sensor platform has the potential to support the development of smart food labels.

Envisaged internal collaborations

This contribution involves ongoing collaboration with TCVB groups specializing in sensor fabrication, food and analytical chemistry, and paper-based materials, represented among the co-authors.

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A Zeolitic Imidazolate Framework Phase with Broad Compatibility for Protein Encapsulation

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Encapsulation of biomolecules within porous materials offers an effective strategy to enhance their stability and broaden their utility under non-native conditions.[1] Among these materials, zeolitic imidazolate frameworks (ZIFs) have emerged as promising hosts owing to their biocompatibility and facile aqueous synthesis. Protein encapsulation in ZIFs is typically achieved through biomimetic mineralization, whereby non-covalent interactions between proteins and metal ions promote framework nucleation and growth.[2] Consequently, current ZIF-based encapsulation strategies predominantly favour proteins with low isoelectric points (pI), whereas proteins with high pI values remain difficult to incorporate because electrostatic repulsion can hinder framework formation. Here, we identify a ZIF phase, denoted **U12**, that enables broad-spectrum protein encapsulation across a diverse range of physicochemical properties. High encapsulation efficiencies were achieved for proteins spanning an exceptionally wide pI range, from pepsin (pI $\approx$ 1) to lysozyme (pI $\approx$ 11). Structural characterization by electron diffraction revealed the crystallographic features of **U12**, while systematic variation of synthesis parameters, including ligand-to-metal ratio and stirring conditions, together with turbidity analysis, provided insight into its formation pathway. Beyond its broad protein compatibility, **U12** exhibited excellent phase stability in organic solvents such as ethanol, highlighting its robustness under processing and application-relevant conditions. As a proof-of-concept application, glucose oxidase (GOx) was encapsulated within **U12**, yielding biocomposites with enhanced resistance to urea-induced deactivation and demonstrating the protective capability of the framework toward enzymatic function. By overcoming charge-related constraints, **U12** substantially expands the accessible protein space for framework encapsulation. Furthermore, the discovery of **U12** enlarges the design space of biomolecule-directed framework formation and opens new opportunities for integrating diverse biological functions into porous crystalline materials.

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Mechanochemical Synthesis of Hydrogen-Bonded Organic Framework and Enzyme Biocomposites for Biocatalysis

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Hydrogen-bonded organic frameworks (HOFs) are porous materials with growing relevance for sensing, catalysis, and biocatalysis.[1] They arrange into a three-dimensional porous network made from aromatic organic linkers featuring hydrogen-bonding functional groups that interact via directional hydrogen bonds and π–π stacking interactions. Their mild synthetic conditions and protective porous environments make them attractive platforms for enzyme immobilization, where maintaining enzyme activity and stability is essential. However, conventional one-pot solution synthesis often results in rapid crystallization, limiting control over crystal growth and leading to uneven enzyme distribution, with enzymes predominantly located near the crystal surface. [2-4] Recent work has shown that combining mechanochemistry with NH_3-vapor-assisted aging can improve enzyme loading, promote a more homogeneous enzyme distribution, and enhance catalytic performance in BioHOF-1 enzyme biocomposites. [5] Building on this strategy, this project investigates the mechanochemical synthesis of new HOF–enzyme biocomposites using extended organic ligands designed to increase framework pore size. Larger pores may improve substrate accessibility, conversion, and reaction kinetics, but must be balanced against the need to maintain framework integrity and enzyme stability. By exploring the relationship between ligand length, pore structure, enzyme incorporation, and catalytic performance, this work aims to expand the design principles for HOF-based enzyme biocomposites and contribute to the development of more efficient porous materials for biocatalysis.

Envisaged internal collaborations

Given the interdisciplinary nature of the project, which integrates crystal engineering and enzyme immobilization, collaborations with research groups in particle technology and biotechnology are in place or planned. These include the Institute of Process and Particle Engineering, the Institute of Biotechnology and Biochemical Engineering and the Institute of Molecular Biotechnology, whose expertise will support the development and application of the proposed research.

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Cellulose Nanofibers from Wood Pulp via Enzymatic Pretreatment and High-Pressure Homogenization

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Nanofibrillated cellulose (NFC) is a cellulose-based material with fiber lengths larger than 100 nm and diameters less than 30 nm [1]. There are several methods for NFC production, among them enzymatic treatment, high-pressure homogenization, ultrasonication, or combinations of thereof [2]. This study investigates the properties of NFC produced in the > 100 g scale by continuous high-pressure homogenization of enzymatically pretreated pulp, using a GEA Lab Homogenizer Panther 3006. The pulp is treated with cellulase enzymes for different durations, followed by homogenization at different pressures and numbers of cycles. Elaborate photometric assays and statistical analysis tools are used to determine the influence of the processing parameters on the resulting NFC properties. The results obtained deepen our understanding of the factors that control the properties of NFC produced through continuous, high-pressure homogenization. The methods developed give access to well defined, reproducible NFC gels suitable for extrusion 3D-printing, coatings and beyond.

Figure 1. Process scheme and homogenization equipment

Envisaged internal collaborations

The work is a collaboration of BPTI, IBioSys. Future collaboration with biotechnologists working on cellulases or biotechnological fibre production could further our understanding of the targeted enzymatic disintegration of cellulose fibres, and could lead to optimized nanocellulose yield, properties and innovative applications.

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