Designing of biocatalysts utilizing ionic liquids and tunable carriers in model chemical processes

The main goal of this work is to develop novel supports for enzymes that enhance the overall properties of the biocatalyst. The catalytic performance of novel materials will be demonstrated in model chemical processes for the production of fine chemicals, as well as high-value-added products derived from biomass. The novelty of the project is focused on the use of modern materials with tuneable surface morphology, and the modification of their surface with ionic liquids (IL) with unique properties to obtain highly active, selective and moreover stable biocatalysts. Additionally, studies on activity and stability of immobilized lipases in deep eutectic solvents (DES) will be performed. The stability of biocatalysts during the flow or batch process with consecutive cycles is a crucial factor that impacts the economic feasibility of the overall method.

The chemical industry is undergoing a transformation driven by the growing interest in sustainable technologies. To achieve the goals outlined in the 2030 Agenda for Sustainable Development, the industry is focusing on advancing chemical processes with minimal environmental impact. This includes using recyclable and selective catalysts, avoiding toxic reagents, reducing energy consumption, and minimizing waste and solvent usage. One promising approach is the use of heterogeneous catalysts, which offer several advantages. These catalysts can be easily separated from the reaction mixture, allowing for efficient recycling. They also improve the mechanical and thermal properties of the process. Solid catalysts are particularly well-suited for continuous-flow technologies, which significantly enhance process efficiency.

In the realm of biotransformations, heterogeneous biocatalysts have emerged as a successful combination of various benefits. Proteins possess unique properties such as high selectivity, activity, and biodegradability, making them ideal catalysts. However, enzymes often require stabilization methods to ensure their long-term sustainability.

In our research, we are exploring the potential of using commercially available enzymes, specifically lipases, for various applications. These enzymes, such as lipase B from *Candida antarctica* or lipase from *Aspergillus oryzae*, will be immobilized on specially designed solid supports modified with ionic liquids (IL) or stabilized in deep eutectic solvents (DES) *e.g.,* choline chloride-glycerol.

We aim to understand how the liquid structure of ILs relates to their properties, such as their compatibility with reactants and their ability to stabilize enzymes. By leveraging this knowledge, we can design an optimal surface modifier for the solid support. Previous studies have shown that both enzyme immobilization and the inclusion of ILs in the catalytic system enhance the activity, thermal and mechanical stability of enzymes.

To achieve this, we employ a technique called supported ionic liquid phase (SILP), where a thin film of IL is formed on the solid support matrix. This can be achieved through either physical adsorption or chemical bonding of the IL. SILP materials offer the advantages of both homogeneous and heterogeneous catalysis, resulting in improved enzyme stability and performance.

In our project, we are focusing on designing suitable carriers for enzymes, which is a crucial aspect of our research. We are exploring the use of innovative materials, including electro-spun polymers, inorganic silica materials and coconut shell activated carbon as a potential carrier. To enhance the performance of these carriers, we will immobilize environmentally friendly and readily biodegradable ILs based on glucose onto their surfaces. The selected enzymes will then be adsorbed onto the IL-modified carriers, forming what we call bio-SILP catalysts. These bio-SILP catalysts are expected to exhibit high selectivity and activity.

In the final phase of the project designed bio-SILP catalysts will be tested in biomass-derived chemicals biotransformation and fine chemicals synthesis. Biomass-derived chemicals, such as α-angelica lactone and furfuryl alcohol derivatives will be transformed to alkyl levulinates and furfuryl alcohol esters in the bio-SILP presence.