From Catalysis to Circular Materials: Sustainability-Driven Research

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Motivation

Sustainable chemical production requires high efficiency, minimal byproducts, and the avoidance of hazardous contamination. At IIT Hyderabad, we aim to design catalysts based on earth-abundant metals to enable environmentally benign processes. Our research work bridges the intersection of chemical innovation and sustainability, focusing on how fundamental inorganic/organometallic chemistry can align with sustainability aspirations. Rather than being limited to traditional "applied environmental science," we embed sustainability at the molecular level by innovating cleaner, safer, more efficient chemical routes. Our work spans catalyst design, polymer chemistry, and organic synthesis — all with an eye on minimizing environmental impact and maximizing atom economy, resource efficiency, and safety.

Challenges and solutions

The main areas that we are working on focus on Earth-abundant metal catalysis for "green chemistry. Instead of relying on expensive or toxic metals, our work focuses on earth-abundant, non-toxic, and cost-effective metal complexes based on alkali metals, alkaline earth metals, titanium, zirconium, aluminium, and zinc, which shine as sustainable and affordable alternatives to precious metal catalysts, providing a crucial solution to our environment and resources, particularly in large-scale organic transformations. Second, in line with the principles of green chemistry, atom-economical and selective transformations, such as the research on hydroboration of unsaturated bonds (alkenes/alkynes), strive for high selectivity and low waste. Although the area has been dominated by transition metal complex catalysts, main-group element complexes have been making a steady but essential influence. Notably, the idea of substituting costly transition metals with inexpensive, non-toxic, and earth-abundant main-group elements has emerged as a promising new direction in organometallic chemistry. Recent developments in ring-opening polymerization (ROP) and the copolymerization of cyclic esters, epoxides, and anhydrides have utilized benign metal catalysts. Homogeneous alkali and alkaline-earth metal complexes (Li, Na, K, Cs, Mg, Ca, Sr, Ba) have proven effective for polymerizing cyclic esters. When designed carefully, these polymers offer a sustainable option, as they can be produced in biodegradable forms. We are also exploring metal-free and green-solvent approaches, which offer a cleaner and more sustainable alternative to conventional, often hazardous, reaction conditions.

Differentiating factor

Many organic scaffolds vital to catalysis also serve as essential motifs in pharmaceuticals, agrochemicals, and pesticides, with their metabolic stability supporting broad applications in chemical biology. Therefore, a significant challenge lies in developing efficient and sustainable routes for synthesizing bioactive organic scaffolds such as N-methylated amines, which are key building blocks in numerous pharmaceuticals and also function as important amine-protecting groups. We have developed a new methodology where amidophosphine boranes serve as valuable reducing agents, distinguished by their air and moisture stability, as well as their cost-effectiveness. Employing these compounds, we established an environmentally benign and sustainable method for converting carbamates into N-methyl amines under mild, catalyst-free conditions. We are also actively engaged in developing new eco-friendly solvents, which have become a vital component of modern green catalysis. Deep eutectic solvents (DESs)—mixtures of two or three components primarily associated through hydrogen bonding—offer an economical, recyclable, and environmentally friendly reaction medium.

Recently, we developed a DES composed of a quaternary diammonium salt (QDAS) and urea (1:2), which has proven to be a promising and straightforward catalytic medium for the atom-economic synthesis of oxazolidinone compounds from epoxides and isocyanates. In this protocol, no additional catalyst or organic solvent is required, as the DES itself functions both as the solvent and as the catalytic system. Using this method, a diverse range of oxazolidinone derivatives has been obtained in good to excellent yields.

In the area of polymerization, the use of non-toxic metals as ROP initiators provides notable benefits over other metal catalysts. In our work, we demonstrated the fast and efficient ring-opening homo- and copolymerization of cyclohexene oxide and glutaric anhydride employing a titanium promoter in solvent-free conditions. Titanium is an excellent choice for the ring-opening polymerisation (ROP) of cyclic ethers, thanks to its strong catalytic activity, affordability, and non-toxic properties. This makes titanium-based catalysts ideal for producing biodegradable polymers for applications such as drug delivery and medical implants. With rising environmental awareness, scientists are now focusing more than ever on creating biodegradable materials to replace harmful non-biodegradable ones.

Next phase of the work:

Our current focus lies in designing new ligand systems suitable for a variety of catalytic transformations, including the hydroboration of nitriles, alkynes, and carboxylic acids; ketone cyanosilylation; cross-dehydrocoupling of amines and silanes; and the synthesis of urea, biuret, isourea, isothiourea, phosphorylguanidine, and quinazolinone frameworks.

We also plan to focus on modifying DESs by adjusting the hydrogen bond donor (HBD) and acceptor (HBA) components, as well as their ratios. Doing so will allow us to adjust properties such as viscosity, density, melting point, and polarity to match the specific needs of various reactions. This tailored design will help us create more efficient and sustainable DES-based systems for a wide range of organic catalytic reactions. Depolymerization is a promising strategy for recycling waste plastic into constituent monomers. Polyurethane, primarily produced through the polyaddition of polyols and polyisocyanates, ranks as the sixth most manufactured polymer and is utilized in a wide array of products, including clothing, furniture, adhesives, insulation, and automobiles. The rising demand for PU products heightens concerns about the disposal of PU waste. In our lab, we are developing a method to depolymerize various types of PU waste, such as PU foams (both rigid and flexible) and elastomers, to recover polyol products. These can be reused in the production of PU products or other valuable items, leading to a circular economy.

Best poster award to Ms Shweta Sagar

Best poster award to Ms Priyanku Nath

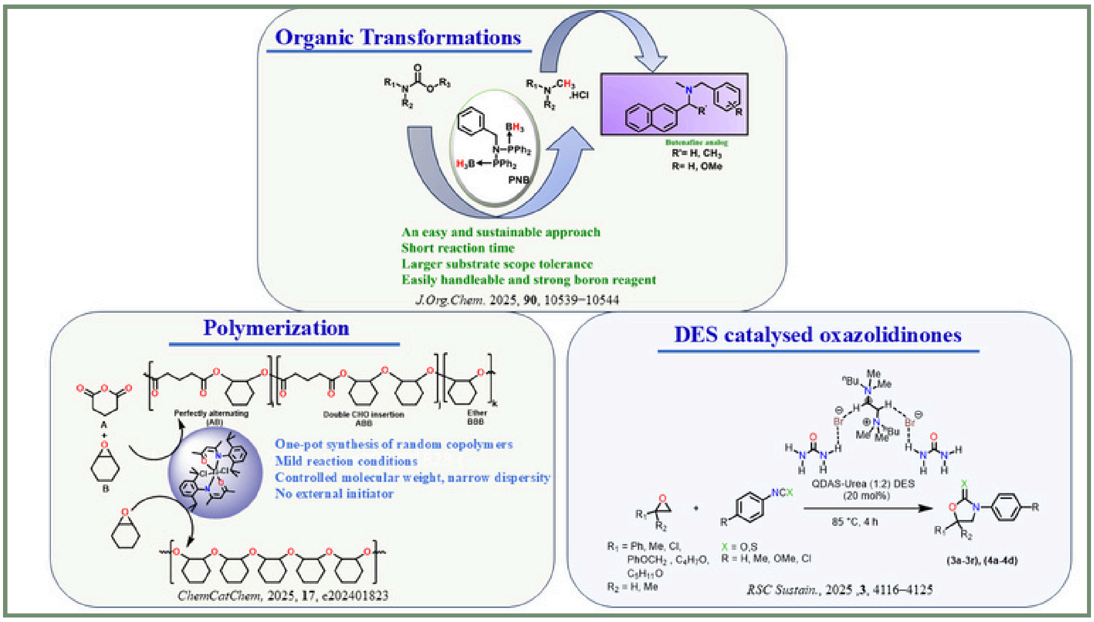

Figure 1. Schematic Diagram of Catalysis by Synthetic Organometallic Chemistry and Catalysis Lab (SOMCC Lab)

"SOMCC Lab" at the Department of Chemistry @IITH

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