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Elevating the C_2 to C_4 Chemistry

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Abstract

In current times, implementing bio-based materials into the chemical value chain is both highly desired and necessary to reduce the greenhouse gas emissions and the carbon footprint of the sector. In this context, using bio-mass derived ethanol has received a lot of attention. Besides its direct application as a fuel additive, ethanol is increasingly recognized as a promising building block for bulk chemicals such as 1-butanol, acetic acid, and 1,3-butadiene, also from an economic perspective.

In the upgrading sequence of ethanol to value-added chemicals, the first step typically involves the dehydrogenation of ethanol to acetaldehyde. With the emerging potential of the hydrogen economy, this route might even become economically advantageous over the state-of-the-art *Wacker-Hoechst* process. Starting from ethanol derived acetaldehyde, *Guerbet* or aldol pathways follow. Despite the availability of tailor-made homogeneous catalysts, *Guerbet* reactions struggle to achieve high yields towards the respective C_4 compound. The selective aldol condensation of acetaldehyde to crotonaldehyde is equally challenging.

To overcome these challenges, we have developed an efficient, mild, selective and scalable process to convert acetaldehyde, into acetoin, using *N*-heterocyclic carbenes as catalyst. Acetoin, a valuable flavouring compound that is usually prepared *via* fermentation from various biomass sources, can be upgraded into valuable C_4 chemicals like butenes, butanediol, and dioxolanes. These value-added compounds can be used in sectors such as chemicals, pharmaceuticals, and materials.

Utilizing a chemo catalytic, solvent-free approach, we have achieved complete elimination of the need for water, enzymes, and cofactors which currently contribute to the high cost of bio-based acetoin and limit its widespread industrial use. Instead, we employ a recyclable, metal-free solid catalyst that converts acetaldehyde, which is readily available from the established bioethanol infrastructure, into acetoin in a highly selective and efficient manner. This innovation not only simplifies the acetoin purification process but also significantly reduces waste water treatment and purification costs.

In summary, we are addressing a significant gap in the current chemical production landscape by potentially making the large-scale production of acetoin both economically viable and environmentally responsible, starting from bio-ethanol derived acetaldehyde as C_2 building block. This development paves the way for its integration into a diverse array of sustainable chemical value chains, ranging from fuels and solvents to polymers and plastics.