Crystal Phase Effects on the Gas-Phase Ketonization of Small Carboxylic Acids over TiO_2 Catalysts


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Invited for this month's cover is the group of Pieter Bruijnincx from Utrecht University. The image shows an imaginary police line-up of two molecules suspected to be involved as intermediates in the catalytic ketonization reaction. Based on the evidence collected, depicted on the pinboard on the wall, the scientist discusses the impact of all this with somebody interested in catalysis that converts waste, wastewater-derived volatile fatty acids in this case, to value-added circular chemicals.
The Full Paper itself is available at 10.1002/cssc.202100721.

What inspired you for the cover image?

In general, the work of a scientist is similar to the work of a detective: you build hypotheses and try to collect sufficient evidence to prove or disprove them. For catalysis research, this requires combining catalytic performance studies with probing the system under working conditions with operando spectroscopy, for example. In this paper, we studied the effect of TiO_2 catalyst type on activity and tried to link this performance to the nature of the species adsorbed on the catalyst surface (i.e., the suspects lined up). Rutile was identified as the best catalyst, depicted by it taking center stage on the evidence board. At the same time, there is not yet a final answer on its major accomplices, the carboxylates in the line-up.

What aspects of this project do you find most exciting?

While this paper focuses on the details of catalytic carboxylic acid ketonization, identifying rutile as highly active polymorph and providing insight into the reaction's mechanistic details, the project this research was part of aimed to more broadly study the challenges associated with recycling carbon in waste streams. This is inherently an interdisciplinary topic. In this case we collaborated closely with separation scientists from the University of Twente, who developed technology to efficiently extract volatile fatty acids from fermentation broths, after which we aimed to valorize these by catalytic conversion, making (precursors for) fuel components, lubricants, or alkylated aromatics. Zooming out more, these efforts were part of a public–private research program that covered the entire chain, from wastewater treatment and fermentation to chemical building blocks synthesis. Connecting different scientific disciplines and working with partners outside academia, in this case the wastewater treatment company Paques, is indeed needed to tackle these major sustainability challenges.

What do you consider exciting developments in the field?

Achieving carbon circularity in chemicals production requires us to use sustainable carbon as virgin feed at the front end, but also to explicitly include end-of-life considerations in the processes we develop. This can be by considering recycling options or, as done in this case, by working on capturing and reusing the carbon contained in wastewater streams. Such circular chemistry efforts require us to reconsider our chemical conversion approaches and molecular design principles, to take a broader systems view of the issue at hand and to collaborate across borders. It's exciting to be able to contribute to these important developments.

Who designed the cover?

The cover was designed by Thomas Hartman, THIS (www.thisillustrations.com).

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