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Lewis, Louis or Luis? The differences and similarities in CO2 assisted propane dehydrogenation with In, Zn and Ga Lewis acid catalysts

Aim

Development of Lewis acid-based catalysts for CO_2 -assisted oxidative propane dehydrogenation and understanding of their function

Justification

CO₂-assisted oxidative propane dehydrogenation (CO₂-OPDH) is heavily researched at universities and in industry. A commercially viable catalyst is yet to be discovered and developed, with major issues in selectivity and stability remaining. Even though it is an oxidative reaction, Lewis acid active sites seem to perform well for this reaction. Promising results were achieved with supported indium, zinc, and gallium materials. Such catalysts could help replace the current technologies for propylene technologies, with low catalyst stability, poor per pass conversion, and toxic and pricey catalysts. In this thesis we will dig a deeper into how and why these types of catalysts hold promise, to derive avenues for better catalyst design.

The mechanism(s) by which supported Lewis acids catalyse OPDH are strongly debated, and seem to vary with catalyst composition and structure. Likely, a redox active support is needed for CO_2 activation, and the Lewis acid site facilitates hydrogen abstraction. In this thesis, you will hunt for the underlying elementary surface reaction and their kinetics to reveal the catalyst's essential properties. You will derive these by comparing different metals on different support materials. Through product analysis and synthesis-structure-activity relationships you will come to understand the inner workings of OPDH catalysis. A combination of kinetic tests and operando spectroscopy will be essential to achieve this.

This thesis offers an excellent opportunity to be trained in applied catalysis, covering synthesis, kinetics, some characterisation, and catalytic testing on particularly relevant catalysts. Ideally you will approach the problem from both the fundamental and the applied perspective, trying to use the former to achieve the goals of the latter.



Program

- Literature study bringing together the guiding principles for Lewis acid catalysed (O)PDH
- Synthesis of Ga, In, Zn active sites on a selection of support materials
- Catalytic testing under relevant PDH conditions and probing the effect of adding CO2
- Deeper mechanistic investigation with operando IR spectroscopy, isotope experiments, ...

