LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	**Supervisor(s)**	**Funding**
Ir. Lennert D'ooghe	Prof. Dr. Kevin Van Geem Prof. Dr. Vladimir Galvita	

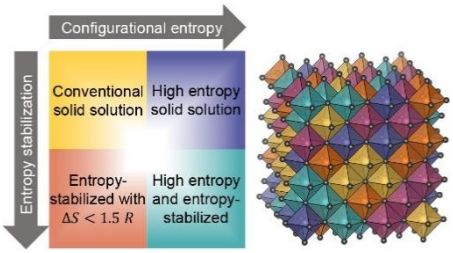
Combined experimental and computational evaluation of high entropy oxide catalysts through Temporal Analysis of Products (TAP)

Aim

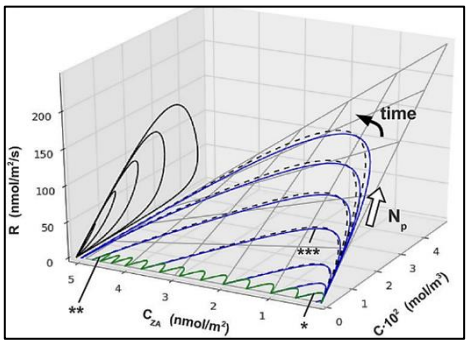
To synthesize and test transition-metal-based high entropy oxide catalysts for CO_2-assisted propane dehydrogenation, leading to structure-performance relations. A particular focus lays on Temporal Analysis of Products (TAP) as experimental and computational kinetic characterization technique.

Justification

Propylene is among the most important chemical building blocks in industry. Its main on-purpose production stems from propane dehydrogenation (PDH). Recent research focusses on introducing CO_2 to this system (CO_2-assisted PDH), holding potential to greatly improve the PDH process while simultaneously providing a way for CO_2 utilization. However, the presence of CO_2 introduces a redox environment for which a stable and selective catalyst remains to be found.



Due to their redox properties, transition-metal-based oxides are catalyst candidates for CO_2-PDH. Especially high entropy oxides have great potential due to geometric and electronic effects between the oxide matrix and the active element. However, little is known about their structure-performance relations for CO_2-PDH, impeding their further development. To advance the knowledge herein, LCT's Temporal Analysis of Products (TAP) reactor setup serves as a unique kinetic characterization tool. Through the combination of molecular beam scattering methodology and the mathematical approach of relaxation theory, mechanistic insights of the gas-solid interaction can be obtained with millisecond time resolution. Combining experiments with the Y-procedure – a mathematical approach developed for TAP – allows to decouple diffusion-reaction phenomena and to extract values for non-steady-state chemical transformation rates.



Top: *Sketch of a high entropy oxide. (J. Am. Chem. Soc. 145 (2023) 5991–6006).*
Bottom*: Example of non-steady-state rate/composition space trajectories in TAP. (Chem. Eng. Sci. 66 (2011) 6441–6452).*

Program

- Literature study on high entropy oxides in view of CO_2-PDH.
- Synthesis of a selection of potential high entropy oxide catalysts for CO_2- PDH.
- Characterization of catalysts through N_2-physisorption, TPR, TPO, TPD, SEM-EDX, etc.
- Activity screening in LCT's step response reactor (PFR).
- TAP experiments on (a selection of) most performant sample(s).
- Extracting diffusion rates and chemical transformation rates from the experimental TAP data, using the Y-procedure.

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