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DESIGN OF INDIUM OXIDE CATALYSTS FOR SUSTAINABLE METHANOL PRODUCTION FROM CARBON DIOXIDE

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Project Summary: The use of CO_2 as a chemical feedstock is pursued to mitigate global climate change while fulfilling the growing demand for green products, with its thermocatalytic hydrogenation to methanol comprising one of the most advanced routes. Within this doctoral research, precision catalyst synthesis, advanced characterization and computational methods, and accurate testing were applied to gather fundamental understanding of In_2O_3 as a breakthrough catalyst for this transformation. The insights gained led to improved catalyst formulations that are considered for pilot demonstration by the energy firm Total. In-depth mechanistic analysis identified limited hydrogen activation ability as well as water-driven sintering as limitations of bulk In_2O_3. The former was overcome by introducing minimal amounts of palladium or nickel in precisely engineered architectures, unlocking promotional effects while curtailing detrimental intrinsic hydrogenation properties. The latter aspect was addressed by supporting In_2O_3 on monoclinic zirconia which enabled high and resilient dispersion, while further boosting activity via the formation of additional active sites on In_2O_3 and at the oxide boundaries. Thermodynamic and kinetic drivers for the application of the materials developed in a methanol-based hydrogen storage technology were explored, and finally, rigorous process modelling demonstrated bright techno-economic perspectives for CO_2-based methanol synthesis and, more relevantly, its absolute planet-wide sustainability.

CV. M.S. Frei obtained his BSc in Chemical Engineering in 2014 and his MSc in Chemical and Bioengineering in 2016 at the ETH Zurich. In the same year, he started his PhD in the frame of an industrial collaboration with Total Research & Technology Feluy in the Advanced Catalysis Engineering group led by Prof. J. Pérez-Ramírez.