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CATALYTIC PROCESSES FOR INTENSIFIED VINYL CHLORIDE PRODUCTION

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Project Summary: In the context of PVC production, a more sustainable process for one-step vinyl chloride (VCM) manufacture is intensively sought after. In this quest, three major milestones are: *i*) development of more robust ethene oxychlorination catalysts, *ii*) process intensification *via* elimination of energy intensive dehydrochlorination of intermediate ethylene dichloride (EDC), and *iii*) feedstock change from ethene to the more abundant ethane. This thesis addresses these aspects by development of new catalysts and corresponding mechanistic understanding by evaluation of catalytic performance and reaction kinetics, combined with molecular level modeling. In particular, bulk CeO_2 and EuOCl were identified as stable oxychlorination catalysts, in addition enabling direct VCM production with yields up to 25%. Mechanistic understanding of the reaction network ultimately enabled to overcome their limitations (by-product formation, low activity) by nano-structuring, separating catalytic oxychlorination and dehydrochlorination functions, and optimizing the reactor configuration. The developed CeO_2/ZrO_2-Ca/Al_2O_3 system led to > 98% VCM selectivity (2% EDC) with a 4-fold increase in productivity compared to EuOCl. In contrast, ethane oxychlorination on a broad range of materials primarily yielded ethene instead of VCM as a consequence of active site competition, intrinsically hampering the use of ethane as feedstock for VCM production.

CV. M. Scharfe obtained his BSc in Mechanical Engineering in 2013 and his MSc in Process Engineering in 2015 at ETH Zurich. After conducting his master thesis in the group of Prof. Dr. Javier Pérez-Ramírez, he continued with his doctorate in the same group.