SINCHEM PhD subject

Synthetic Strategies for Hydrocarboxylation of Bifunctional Substrates

The world is facing some Grand Challenges in the near future. Resources are becoming increasingly scarce, while the population is increasing. Societal needs require addressing the sustainable supply with energy, materials and water. This project shall contribute to solving one of these Grand Challenges that our society is facing: the change from a fossil fuel-based society to a society based on sustainable use of renewable feedstock.

One of the most abundant renewable resources of carbon is carbon dioxide (CO_2). Due to the implementation of carbon capture technologies, enormous quantities of CO_2 are separated from exhaust streams and available as potential feedstock for the chemical industry. Such chemical exploitation of CO_2 aims to generate value by producing chemicals and materials. Our vision is to create an anthropogenic CO_2-loop, where CO_2 released at the end of the use-span of carbon-based goods of our every-day life is used in the production of new materials.

This project's aim is to identify new synthetic pathways to carboxylic acids and their derivatives based on the reaction of unsaturated substrates with CO_2 and hydrogen as well as developing novel catalysts with improved activity and functional group tolerance. Existing catalytic systems will be improved and new catalytic systems developed for the hydrocarboxylation of olefins and alcohols.

Since the hydrocarboxylation consists of reverse water gas shift reaction and consecutive hydroxycarbonylation, different transition metals (Rh, Pd, Ru) will be used, also in heterocombination (cooperative catalysis). The combination of heterogeneous and homogeneous catalysts will be considered in collaboration with Lyon. By screening different metal precursors, ligands, additives and reaction conditions, the system will be optimized for various (bifunctional) substrates.

An important aspect is also the mechanistic study of the catalytic cycle. Therefore, especially spectroscopic methods (HP-NMR, HP-IR) will be used to collect detailed information about the catalytically active species.

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Host PI: Dr. Thomas Müller (CAT Catalytic Center)

The host program

Our partners are also invited to use the analysis capabilities at the associated partner "CAT-Catalytic Center", in particular the analysis tools for complex reactions networks, including *in-situ* and *on-line* monitoring to identify new methods for selective, green processes.