Overcoming Technology Barriers with Tailored Catalysts: Design of Molecularly Functionalized Heterogenous Catalysts for Selective Reductions of Biomass-based Materials

Future success in biomass-based economy requires rapid solutions for converting compounds available from biomass to value-added building blocks for materials and for the chemical industry. These rapid solutions can only be obtained by new catalytic methods. These methods need catalysts that do not yet exist.

This multidisciplinary project develops new catalysts for the processing of biomass-based raw materials. Specifically, it aims at the development of selective reduction catalysts since most of the biobased raw materials are highly oxidized, and reduction will render them more useful as building blocks.

The project focuses on the development and design of ligand-modified heterogeneous metal catalysts. The ligands are molecules that adsorb into the metal surface, modifying and amplifying the catalytic efficiency of the solid metal catalyst. In other words, the ligand molecules act as active co-catalysts. Theoretical and experimental studies are focused on co-operation of ligands and the metal, and on the effect of this cooperation on the efficiency and selectivity of reduction reactions.

The teams will bring to the project complementary expertise: The team led by Professor Honkala will focus on density functional theory calculations and the development of structure-reactivity models for the new catalysts. The group of Professor Pihko focuses on synthetic chemistry, including synthesis of ligands for characterization of catalysts and reactivity studies. Based on atomic-level understanding on the properties of the ligands and how they impact the activity and selectivity in studied reactions, the project seeks to obtain key descriptors to facilitate fast optimization and tailoring of catalysts for a variety of reduction reactions relevant to biomass-based raw-materials.

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