Overcoming Technology Barriers with Tailored Catalysts: Design of Molecularly Functionalized Heterogeneous Catalysts for Selective Reductions of Biomass-derived Materials (FunCat)

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 aims at development of new catalysts for the processing of biomass-based raw materials. We specifically aim at the development of selective reduction catalysts since most biobased raw materials are highly oxidized, and reduction will render them more useful as building blocks.

The project focuses on the development and even design of ligand-modified heterogeneous metal catalysts. The ligands are molecules that adsorb on 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. The theoretical and experimental studies focus on co-operation of ligands and the metal, and the effect of this cooperation on the efficiency and selectivity of reduction reactions.

The teams will bring their own expertise to the project: the team led by Prof. Honkala will focus on density functional theory calculations and the development of structure-reactivity models for the new catalysts. The group of Prof. 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, we seek to obtain key descriptors to facilitate fast optimization and tailoring of catalysts for a variety of reduction reactions relevant to biomass-based raw-materials.

The experimental research currently focuses on unearthing the most promising substrates for the catalytic reactions and for identifying the factors responsible for selectivity. At present, the computational work is addressing the interaction between ligand molecules and their binding on a Pt catalyst as well as the influence of ligands on a selective reduction of a simple acid.

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