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

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.

Heterogeneous catalysts are industrially the most applicable due to ease-of-handling and easy separation from the product. Optimization of heterogeneous metal catalysts however remains difficult and laborious. In the current project, we propose the use of organic ligands, typically utilized in homogeneous catalysis, for the surface modification of metals.

Surface-modified catalysts reported earlier typically rely on natural cinchona-alkaloids (e.g. quinine). Before attempting any new unknown ligands, we intend to benchmark our experimental set-up. Thus, a series of test reactions with various metals and support materials are being screened. Early transition metals, such as iron, copper, and nickel have been found to be inactive. Palladium, platinum, and rhodium however all give modest to high yields. Interestingly, despite reports of high selectivity using palladium or platinum in combination with quinine, the obtained enantioselectivities have been low with all catalysts. Especially with palladium though, the yield and selectivity seemed to vary significantly depending on the source of palladium.

Rational ligand optimization requires access to broad ligand library. Steric and electronic variation of the previously utilized cinchona-alkaloids is very demanding and for efficient screening, new simplified ligand structures need to be designed. Our initial efforts have focused on ligands that are readily accessed from commercially available materials and allow exploration of vast chemical space.

For a computational study, platinum was chosen as a model catalyst and the ligand employed in calculations was selected based on experiments. Our initial computational efforts have focused on understanding how ligand molecules bind to platinum and interact with each other. Furthermore, we have addressed stabilities of reactant, intermediate and product molecules on ligand-modified platinum.

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