

Overcoming technology barriers with tailored catalysts

Design of molecularly functionalised heterogeneous catalysts for selective reductions of biomass-derived materials

FUNCAT

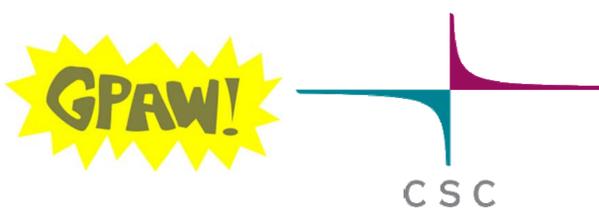
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What is FunCat?

FunCat means Functionalized Catalysts. Catalysts are the engines of chemical reactions. They convert starting materials into products, but are not themselves consumed. But how to design these engines?

2. Methodology

Computational work will employ density functional theory methods (GPAW code). Based on computational results, the structure-reactivity models will be developed for the new catalysts.



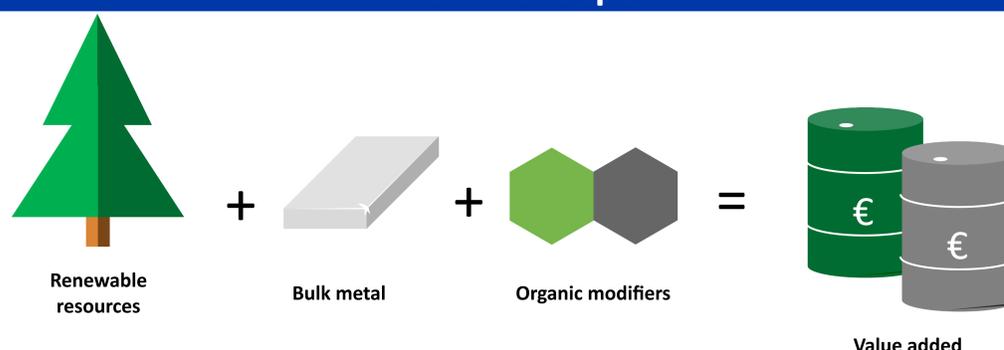
Experimental work involves synthesis of modifier molecules. Their design is based on the computations. The initial designs are refined by the experimental results, and the experiments help to validate the computational models.

The combined result is a refined model that describes how catalyst performance changes by changing the modifiers. These models will lead to accelerated evolution of the catalysts.

Conclusions

We can only solve these problems together!

1. Main concepts



Future: Biomass-based economy, with biomass-based renewable resources. No oil, no fossils.

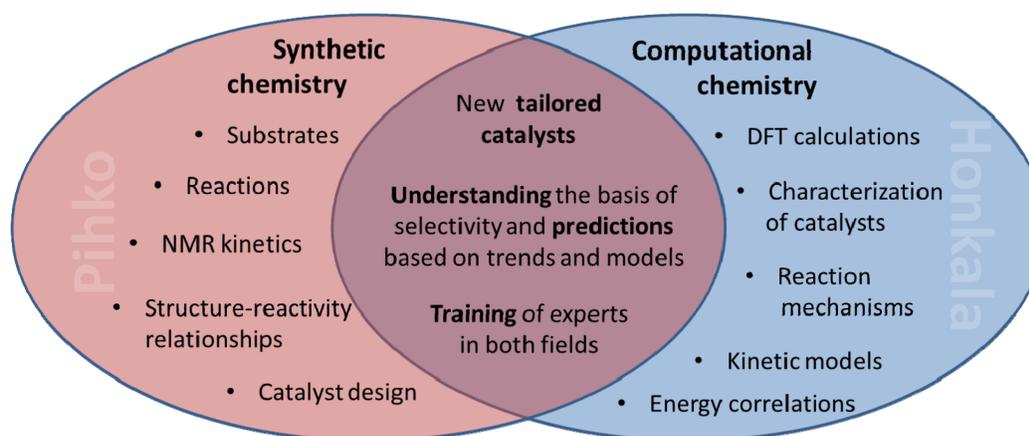
Requires: Rapid solutions for converting biomass to value-added building blocks. These are feedstocks for materials, and for the entire chemical industry.

Catalysts: These are the engines that convert biomass-based compounds to building blocks. They are involved in >80% of all chemical manufacturing. The problem is that **their design is extremely difficult**.

The FunCat solution: We target industrially applicable, supported metal catalysts, but add our own flavor by introducing **tailored modifiers** to improve selectivity and efficiency. We aim at selective reduction catalysts to increase the value of biobased raw materials.

How? Some modifiers for metal catalyst are known, but we do not know how to improve them. Here we will harness the power of computational modeling combined with experimental optimization tools.

3. Expertise of the partners



Acknowledgements



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