

## Accelerating Understanding & Development with Data Mining & Machine Learning

Initiative: Momentum - Förderung für Erstberufene

Bewilligung: 24.06.2019

Laufzeit: 5 Jahre

Projekt-Website: <https://www.schoenebeck.oc.rwth-aachen.de/>

While homogeneous catalysis is arguably one of the key areas to tackle the ever increasing demands of sustainability, energy- and environmentally related questions, it has also transformed the way chemists assemble molecules. However, many challenges exist in the field and the identification of solutions will greatly benefit from innovative approaches. The strategies to develop novel solutions and reactivities in homogeneous metal-catalysis include (i) detailed mechanistic studies and rational developments, (ii) trial-and-error screening approaches, (iii) directed high-throughput screening with modern data-analysis. In the last eight years the group has been active in combined computational and experimental mechanistic studies to develop novel reactivities and solutions in the context of organometallic catalysis. However, the rational design of catalysts and conditions is time-consuming, as it requires in-depth mechanistic insight. To be able to advance those more challenging areas, a multiscale approach will be imperative. The goal is therefore to use data-intense approaches by implementing high-throughput screening facilities and the most modern data mining tools in the context of artificial intelligence and machine learning.

### Projektbeteiligte

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### Open Access-Publikationen

**Accelerated dinuclear palladium catalyst identification through unsupervised machine learning**

