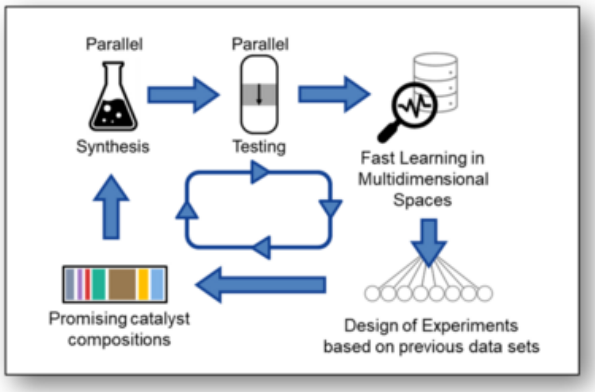
Theory accelerates experiment: Innovative approach saves years of trial and error in the lab



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Scientists around the world are working on the further development of chemical processes to make them more efficient, cost-effective and environmentally friendly. However, the optimization of experiments in the laboratory through to processes suitable for industrial use can take decades since new discoveries are often based on labour-intensive trial and error. The current collaboration between scientists from BasCat (UniCat BASF JointLab) and the theory department of the Fritz Haber Institute aims to put an end to this: They present a systematic approach to experiment design that can speed up the development of new processes significantly. In a study recently published in ACS Catalysis, they demonstrate this using the example of an important chemical reaction, the non-oxidative propane dehydrogenation to propylene.

Propylene is an important feedstock chemical, for example for polymer manufacturing. Its demand is expected to approach 200 megatons by 2030, which cannot be met with the existing cracking processes. More efficient ways of industrial production must therefore be found. However, the development of the process currently in commercial use took more than 40 years!

The key point in improving many catalytic processes - including this one - is the use of so-called promoters. These are substances that increase the catalytic efficiency of a reaction or mitigate deactivation. The discovery of new promoters and their optimization can take years, as potential candidates are tried out and optimized only sequentially. The now presented approach globally explores a multi-promoter design space with only limited experiments: With less than a hundred experiments performed within a matter of weeks, the team at BasCat and the Fritz Haber Institute developed a process for the production of propylene that can compete

with the one commercially used. Their approach is based on an efficient adaptive design-of-experiment planning and a throughput maximization through parallelized testing.

The results not only provide insights into more efficient ways to find multi-promoter formulations, but are also proof of the successful collaboration between BasCat scientists and the Fritz Haber Institute. The collaboration focuses on basic research in the field of heterogeneous catalysis and in particular on the catalytic conversion of hydrocarbons into products with higher added value.

The recent study gas recently been published in *ACS Catalysis*: C. Kunkel et al. Systematic Exploration of a Multi-Promoter Catalyst Composition Space with Limited Experiments: Non-Oxidative Propane Dehydrogenation to Propylene, *ACS Catal.* 2024, 14, 11, 9008–9017, https://doi.org/10.1021/acscatal.4c01740