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Bayesian Optimization of Promoted Pt/Al_2O_3 Catalysts for Perhydro-Benzyltoluene Dehydrogenation

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Liquid organic hydrogen carriers (LOHCs) facilitate safe handling as well es efficient storage and transportation by chemically binding hydrogen under mild conditions in a catalytic hydrogenation. Release of the hydrogen from the non-flammable liquid is realised in catalytic dehydrogenation and provides technological hurdles due to a limiting thermodynamic equilibrium conversion making a compromise between activity, selectivity and stability of the catalysts as well as the LOHC inevitable. The catalytic properties can be improved by the addition of promotors, which often follows a volcano-type behaviour [1], i.e. a beneficial effect is observed until an optimum loading is reached, while higher loadings are detrimental. For such optimisation processes, Bayesian optimisation (BO) provides a tremendous potential for data-driven identification of promising catalyst compositions in a multidimensional parameter space.
Herein, multi-promoter systems serve as a primary application example for a data-driven approach towards catalyst development. BO is leveraged to navigate through the high-dimensional parameter space of catalyst design. Traditional trial-and-error experimentation is replaced with a BO approach, while the study aims to systematically identify promising metal and promoter loadings while minimising the experimental workload. The practical workflow involves data integration and validating existing datasets while performing first experiments to establish a robust "first generation" of catalyst data using various combinations of 11 promoters. This work focuses specifically on the compositional design space of the Pt/Al_2O_3 catalyst, where up to four promoters must be selected from a pool of 11. The global optimum and broad coverage of the parameter space are targeted alike. A multi-objective optimization approach is used for maximizing hydrogen release and minimising side product formation. Eventually, preparation and experimental testing of the BO-proposed catalyst generations is conducted to validate the proposed candidates. Ultimately, this work seeks to establish a data-driven, precise methodology for material optimization, accelerating the development of efficient LOHC dehydrogenation catalysts.

[1] Domenic Strauch, Pia Weiner, Bidyut B Sarma, Andreas Körner, Elisabeth Herzinger, Patrick Wolf, Anna Zimina, Andreas Hutzler, Dmitry E Doronkin, Jan-Dierk Grunwaldt, Peter Wasserscheid, Moritz Wolf, Bimetallic platinum rhenium catalyst for efficient low temperature dehydrogenation of perhydro benzyltoluene, 2024, Catalysis Science & Technology, 14, 1775-1790.