



## Bimetallic Platinum-Rhenium Catalysts: Enhancing Hydrogen Storage Efficiency through Material Optimization and Synthesis Modification

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### Significance and Relevance

Dehydrogenation performance and productivity of Pt-Re catalysts are significantly influenced by the support material's composition, morphology, and surface chemistry. Novel insights include the identification of charge effects and interactions between the precursors of the two metals and between metal precursors and support material as critical factors. Additionally, the research highlights the impact of metal loading and synthesis procedures on catalyst activity, providing a comprehensive understanding of the optimization of these variables to enhance the hydrogen storage efficiency in LOHC systems.

*Preferred and 2<sup>nd</sup> choice for the topic:* Fundamental advances in understanding catalysis or H<sub>2</sub> storage and transportation

*Preferred presentation:* Oral preferred or Short Oral

### Introduction and Motivations

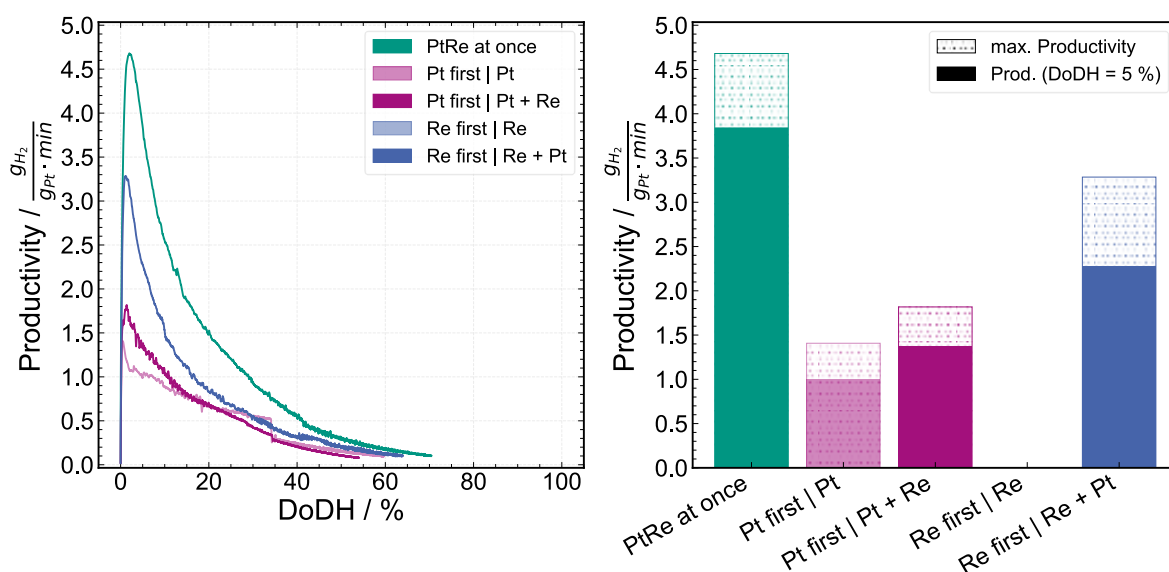
Hydrogen as an energy carrier offers many benefits for the environment, energy security, economy, and end users.<sup>1</sup> However, cost-effective, compact, safe, and convenient storage of hydrogen are essential for large-scale implementation. Further, the volumetric energy density of hydrogen is low compared to other energy carriers.<sup>2</sup> One approach to address this challenge is the use of liquid organic hydrogen carriers (LOHCs) for chemical hydrogen storage. LOHCs are liquids that can chemically bind hydrogen in a reversible manner, which allows for long-term storage and safe transportation of hydrogen under ambient conditions.<sup>3,4</sup> Benzyltoluene/perhydro benzyltoluene (H0-BT/H12-BT) is a technical relevant LOHC system that is thermally stable, has a low toxicity, and has wide liquid range. It has a hydrogen storage capacity of 6.2 wt.%, which is equivalent to 2.1 kWh kg<sup>-1</sup> or 1.9 kWh L<sup>-1</sup>.<sup>5</sup> However, to maximize the hydrogen storage capacity and the number of repeated loading and unloading cycles via catalytic hydrogenation and dehydrogenation, respectively, a superior catalyst selectivity and high conversions are of utmost importance. We recently proposed the use of a bimetallic platinum-rhenium catalyst system, which shows particularly promising characteristics and is therefore an attractive subject for further research.<sup>6</sup>

### Materials and Methods

In this study, the influence of support material and synthesis procedure on the dehydrogenation activity of bimetallic platinum-rhenium (Pt-Re) catalyst systems is investigated. Therefore, a range of supported Pt-Re catalysts were prepared by wet impregnation with strong electronic adsorption and the resulting catalysts as well as the bare support materials were thoroughly characterized by means of inductively coupled plasma atomic emission spectroscopy (ICP-AES), X-ray diffraction (XRD), transmission electron microscopy (TEM) and N<sub>2</sub> physisorption. Porous Al<sub>2</sub>O<sub>3</sub> was used as catalyst support while the boehmite precursor and different calcination temperatures represent a first parameter variation. Further, the procedure for wet impregnation was altered, e.g. by multiple consecutive impregnation steps or by varying the order of the metal precursors applied. Dehydrogenation activity was then evaluated in semi-batch laboratory-scale dehydrogenation experiments to compare key performance indicators, such as the degree of dehydrogenation (DoDH) of perhydro benzyltoluene and the platinum-based productivity of the catalysts.

## Results and Discussion

The dehydrogenation performance and catalyst productivity of the prepared catalysts strongly depends on the utilized supports. These results indicate that the composition, morphology and surface chemistry of the support significantly influence the catalyst activity. This may be linked to charge effects related to the point of zero charge of the support material and the charge of the applied metal precursors. Furthermore, a strong correlation with the metal loading and the synthesis procedure (Figure 1) could be observed. Insufficient distribution of the active metal over the support surface as well as strong interaction with material additives might hamper the catalysts activity. Morphological differences in the support materials, such as mean pore diameter and specific surface area, can additionally influence the activity, for example via pore diffusion limitations. In general, the activity of supported catalysts is based on a complex interplay of various factors, which are extensively examined to provide a better understanding of the underlying effects.



**Figure 1:** Productivity (left) and maximum productivity as well as productivity at a DoDH of 5% (right) during semi-batch dehydrogenation of perhydro benzyltoluene using Pt-Re/Al<sub>2</sub>O<sub>3</sub> catalysts prepared by one impregnation step or two consecutive impregnation steps

The herein presented study provides fundamental insights into the performance of supported bimetallic platinum-based catalysts as a function of the structure and type of utilized support material as well as synthesis procedure. It especially highlights the importance of understanding how different factors can affect synthesis and catalyst activity in order to develop more efficient systems in the future.

## References

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