Adaptive Experiment Planning for Inverse Design and Understanding: Synergistic Interactions as Key to Optimized Multi-Promoter Formulations

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Self-driving laboratories make ever-larger materials design spaces accessible, but experimental throughput remains limited. Exhaustive screening is infeasible, while optimization-focused sampling may locate a promising candidate without explaining why it works or revealing viable alternatives should it later prove unsuitable[1]. For multipromoter catalysts, this distinction matters because performance can depend on interactions that traditional single-promoter studies miss[2, 3].

Here, we combine search and learning for multipromoter catalysts for nonoxidative propane dehydrogenation in a 10-dimensional composition space containing Pt and nine promoters, with 6.08×10^{13} candidate formulations. Our adaptive sampling starts from a simple, interpretable response model and expands it only when new data reveal missing complexity. Each experimental batch therefore improves our understanding of the design space while focusing the search on promising compositions. Parallel synthesis and testing, coupled with automated data analysis, made this accelerated experimental loop practical (Figure 1a).

With 48 adaptively planned evaluations (six weeks of experimentation), we identified a Pt-Sn-K-Ce-Zn formulation near the predicted Pareto front that delivered a higher integrated propylene yield (Y_2) and improved stability (D_2) relative to the Pt-Sn-K industrial reference catalyst (Figure 1b). Removing promoter interactions from the model contracts the predicted performance space so that the Pt-Sn-K reference lies directly on its Pareto front (Figure 1c), seemingly only benefiting from individual promoter effects. Our Pt-Sn-K-Ce-Zn formulation moves beyond this predicted limit through synergistic promoter interactions, including the strong stabilizing interaction between K and Ce identified in this study[3].

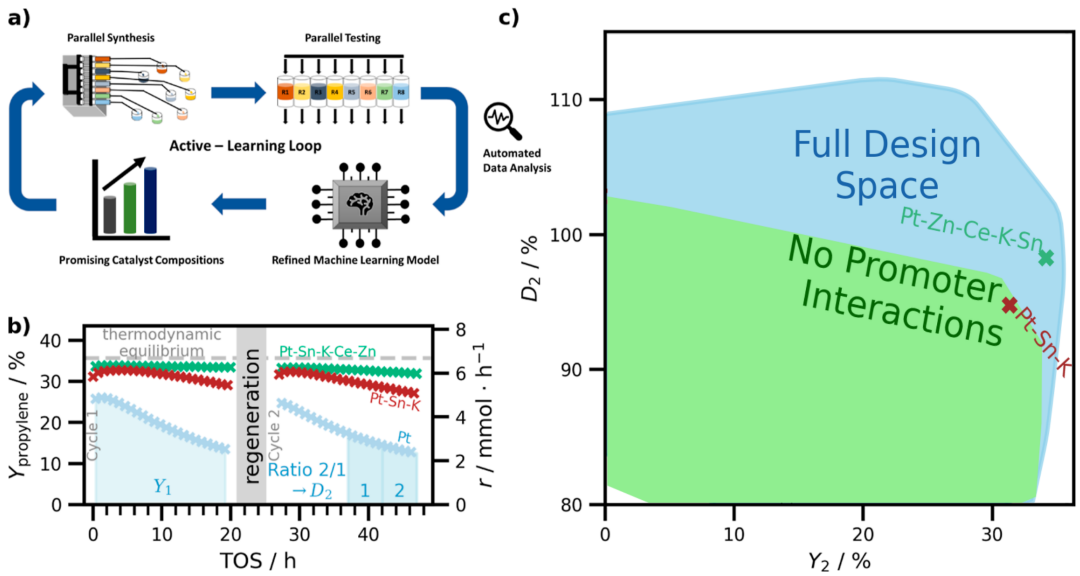

Figure 1: (a) Schematic of the accelerated discovery loop. (b) Reaction yield toward propylene over two PDH cycles of 20 h time on stream with a 4 h regeneration period in between. Shown are the unpromoted Pt catalyst, a Pt-Sn-K reference catalyst, and the novel Pt-Sn-K-Ce-Zn formulation identified here. (c) Predicted yield-deactivation Y_2/D_2 performance spaces for the full model and that model with promoter interactions turned off.

References

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[3] C. W. P. Pare, A. Terzi, C. Kunkel, M. Geske, R. Naumann d'Alnoncourt, C. Scheurer, F. Rosowski, and K. Reuter, *ACS Catal.* **16**, 6798-6807 (2026).