ABSTRACT:

Catalyst Discovery for Ammonia Synthesis Using Active Learning

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Although the literature data on heterogeneous catalysts are high-dimensional, inconsistent, and contain missing data, careful data selection and preprocessing can make them a valuable source for Active Learning (AL) approaches. Adding experimental data via AL allowed the discovery of novel catalyst formulations. Proper feature engineering and selection are necessary for each application to deliver optimal results and gain insights, since each catalytic system may have distinct processes governing catalyst activity, selectivity, and stability. This general framework was employed to discover heterogeneous catalysts for ammonia synthesis, using data mined from the literature and combining domain knowledge with artificial intelligence. The experimental data on conventional thermocatalytic ammonia synthesis catalysts tested in lab-scale fixed-bed reactors were extracted from publications. 936 data points were extracted as data for ML model development. Additional promoted Ru catalysts were synthesized using incipient wetness impregnation. Each catalyst was tested in a four-channel parallel reactor at 30 bar and between 573 K and 703 K. The search space was ultimately selected based on the domain knowledge, where a secondary promoter was varied in a doubly promoted Ru catalyst supported on Pr2O3. Experimental validation showed that predictions from the ML model trained solely on literature data were inaccurate. Integration of additional experimental data via Active Learning (AL) pathways reduced the experimental data required to identify the optimal catalyst by nearly 50% when excluding Ba-containing catalyst data from the literature training set. A path that balances exploration and exploitation of the search space outperformed pathways based solely on exploration or exploitation.