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Optimization of Cu-based Oxide Catalyst for Methanol Synthesis by the Activity Map Envelope Derived from a Neural Network

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The combinatorial approach is a successful tool for material development and for heterogeneous catalyst development. Combinatorial tools were developed consisting of a high-throughput screening reactor using a 96-well microplate, activity mapping by a neural network and optimization by a genetic algorithm. The tools were designed and manufactured to optimize Cu-based oxide catalyst for methanol synthesis. Escape from local optima in the search space is easy by GA, but the efficiency of search is not so high. Instead of GA, a more straight-forward method was applied: all 230, 000 activities of all possible combinations of catalyst components with 5% resolution were predicted by a neural network. These activities were visualized by mapping using two parameters, such as Cu and Zn composition, to find the global optimum.

Keywords: Combinatorial chemistry, High-throughput screening, Genetic algorithm, Neural network, 96 well microplate, Methanol synthesis catalyst

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