High-throughput screening of DeNOx catalysts using self-organizing neural networks

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During the last few years, the development of combinatorial chemistry has enabled to synthesize a large amount of chemical compounds in a short time. High-throughput screening, abbreviated as HTS, has been developed to deal with numerous materials in combinatorial chemistry. However human intervention (trial & error method) in data mining of experimental results lowers the efficiency of HTS.

In this study, the self-organizing algorithm (SOA) of artificial neural networks is applied to the design of DeNOx catalysts. This algorithm can find a near-optimal network which has compact structure and better generalization performance without human intervention. The SOA is used to model relationships between the composition of DeNOx catalysts (Pt, Cu, Fe, and Co) and the catalysis performance (NO conversion). The proposed model is then used to predict the maximum performance of heterogeneous catalysts, thereby accelerating discovery of the optimum composition of DeNOx catalysts.

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