High-throughput screening of DeNOx catalysts using support vector machines

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The combinatorial and high throughput methods were applied to discover new DeNOx catalysts. In this study, the support vector machine (SVM) is applied to predict catalytic activity of various libraries in a quaternary system of Pt, Cu, Fe, and Co supported on aluminium-containing SBA-15 using a self made 64-channel micro reactor. The support vector machine is gaining popularity due to attractive features and promising empirical performance. Compared with traditional neural networks, SVM possesses the prominent advantages of high generalization capability, avoiding local minima, always having solution by a standard algorithm, automatically obtaining network topology structure, and lower workload. The support vector regression is used to model the relationship between the inputs (material composition and reaction temperature) and the output (NO conversion). The proposed model can be accelerating the discovery of the optimum composition of DeNOx catalysts.