

Application of artificial neural networks to catalyst synthesis as a data mining technique

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Many researches are going on in the field of high-throughput experimentation (HTE) techniques in the framework of combinatorial catalysis. Some devices that make such HTE possible are already developed. However, the speedy progress of those experimental tools requires more diverse data mining methods. The objective of data mining is to find relationships between the input and output data obtained from experimentation. In this work, we investigate how artificial neural network (ANN) can be applied to combinatorial catalysis as a data mining technique. First, the relationship between catalytic performances and a broad spectrum of the catalyst elemental composition is derived using ANN. The derived model is then used to predict the maximum reactivity of multi-component catalysts, thereby accelerating the discovery of the optimum composition of catalysts.

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