第400回触媒科学研究所コロキウム

Guided Nanoscale Synthesis and High Throughput Screening for Catalyst Discovery

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The synthesis of heterogeneous catalysts includes the study of large parameter spaces filled with information about relationships between synthesis variables, nano-structure, and catalyst performance. High-throughput (HT) experimentation in combination with theoretical methods, such as statistical design of experiments and density functional theory allows us to study catalysts efficiently and to explore synthesis-structure-reactivity parameter spaces quickly and in detail. Two examples will be presented: 1. Statistical design was used to explore and design cobalt based oxidation catalysts. Emphasis was on the effects of the various synthesis conditions on the nanomaterial properties and activity for oxidation reactions. HT kinetic and spectroscopic data will be presented to demonstrate such a concept. 2. Most of the promoters used industrially for ethylene epoxidation have been discovered through empirical means. The overall HT methodology often relies on a random search of a parameter space to improve catalyst performance. HT systems tend to be very expensive and the random search is not guaranteed to result in an improved catalyst. Advantageous is the combination of the HT approach with a rational catalyst design methodology, which relies on knowledge of the fundamental reaction mechanism that, through experiments in ultra-high vacuum, can be leveraged with density functional theory and microkinetic modeling to predict optimal catalyst formulations. Such an integration of HT with a rational catalyst design scheme for ethylene epoxidation on promoted Ag catalysts will be discussed.

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