第385回触媒科学研究所コロキウム

High-throughput catalyst discovery – From self-healing catalysts forFischer-Tropsch synthesis to LPG production from liquid transportation fuels

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High-throughput experimental (HT), "combinatorial" methodologies are uniquely suited to rapidly generate high quality experimental data, and hence represents the key enabling counterpart to bring computational materials design efforts fruition. The field of catalysis was an early adopter of high-throughput screening technologies, the original Haber-Bosch catalyst, for example, was discovered in 1913 by systematically studying 1000's of potential catalysts before settling on osmium. The advent of powerful computers coupled with the marked success of pharmaceutical companies in novel drug discovery via parallelized synthesis and screening, led to a resurgence of interest in HT catalysis. A brief history of key developments in high-throughput catalysts will be given. Then, two examples for discovery and optimization of catalysts from our group will be discussed.

1) A key problem for all catalytic processes is catalyst deactivation. Normally, catalyst deactivation is addressed by optimizing composition and particle size of the catalysts. Although this may increase catalyst lifetime, most catalysts require periodic off-stream regeneration. In Fischer-Tropsch synthesis (FTS), the primary reaction involves the hydrogenation of CO and polymerization of hydrocarbons. Water is produced in FTS as a side-product. Metallic Co is the preferred catalyst for FTS, however, the presence of water has made it difficult to implement Co. Thus, tuning the redox reaction to favor reduction of the oxide in situ preserves metallic Co under reaction conditions and constitute a key advance in the field of FTS. Kinetic and spectroscopic data will be presented to demonstrate the concept of such a self-healing catalyst based on Conanorods.

2) HT discovery for catalysts for the conversion of liquid hydrocarbon fuels (Kerosene, Diesel, JP-8) into C2-C4 hydrocarbons for portable power applications has led to the deployment of a commercial catalyst. Hundreds of catalysts were screened and transition metal promoted MFI zeolites showed the highest activity. This search involved the systematic investigation of a multi-dimensional correlation between promoter composition, loading, pretreatment/regeneration condition, and the reaction/regeneration rate.

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