Heterogeneous Catalysis Studied by Operand Spectroscopy, Computational Chemistry, and Data Science

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Recent experimental and theoretical studies gave atomic-level insight into heterogeneous catalysis. Nevertheless, the discovery of novel catalysts and catalytic reactions is still a formidable task and, as a result, many of the advances in this area have arisen from trial-and-error investigations. Enormous amount of experimental and theoretical data for heterogeneous catalysis have not yet been integrated into readily searchable databases. Our group has studied Catalysis Informatics based on DFT and machine learning (ML; Figure 1) in combination with experimental studies.[1] Here, I demonstrate case studies on catalyst design by ML-prediction. In the first topic, experimental data for reverse water gas shift (RWGS) reaction by supported metal catalysts are analyzed by ML. After 35 loops of experiment/ML-based prediction cycles, a new catalyst with higher activity than the reported catalysts was developed. In the second topic, ML analysis of DFT data (adsorption energies of CH_3 and CH_2) shows a trend in coking-less alloy surfaces for CH_4 dissociation. Based on the trends, combined with a classical catalysis research using catalytic tests and characterizations, a coking-less dehydrogenation catalyst was developed. Mechism of data-driven catalytic systems is then studied by operando spectroscopic experiments and theory. The combined study shown above may be a standard methodology of catalyst study in near future.

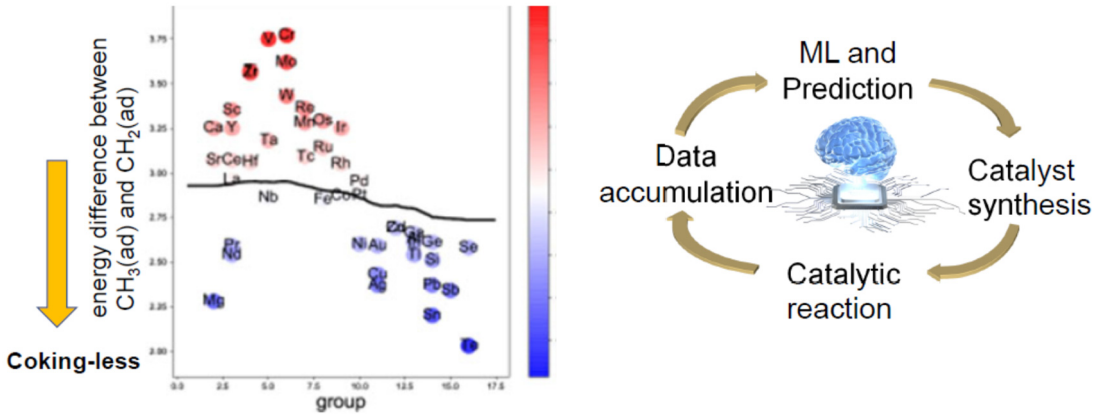

Figure 1 ML-based catalyst design

1) T. Toyao, Z. Maeno, S. Takakusagi, T. Kamachi, I. Takigawa, K. Shimizu, *ACS Catal*. **2020**, *10*, 2260.