Optimizing the distance between two active sites of heterogenous bifunctional catalysts

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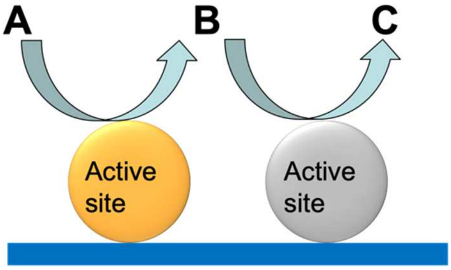

In recent years, multifunctional catalysts have attracted huge attentions in the field of heterogenous catalysis. Such catalysts are thought to be more efficient because they intensify the process by providing multiple active sites for different tandem reactions in one reactor, which eventually helps to save huge amount of energy and resources.

However, there is still a long-going discussion in the scientific community about the structure of these catalysts, of which, distance between different types of active sites is one of the hot topics. In bifunctional catalysts, this distance can play a vital role in defining catalytic activity and the selectivity of the desired product. Shorter distances can lead to metal-ion migration and sintering of the metal particles and longer distance can, on the other hand, result in concentration gradients.[1, 2] There is a need for developing a strategy to predict optimum distance between two different active sites which will eventually help us achieve the maximum performance of the very catalyst.

In this talk, different strategies of design of the catalysts to place the active sites with the defined distance will be discussed with several examples from the already published work supporting the idea of "Distance Matters". This would also include a brief discussion about improving the experimental setup with the input from the mathematical model and improving back the model with the experimental data. The target is to eventually come up with a generalized model which can help us to predict the optimum distance.

Besides this, an overview of challenges in building up a testing facility for high pressure and high temperature gas phase reaction will be discussed and some preliminary results for the proof of the concept will be shown.

[1] Weisz, P. B., Polyfunctional heterogeneous catalysis, *Adv. Catal.,* **(1962)** 13, 137–190

[2] de Jong, K. et al., Nanoscale intimacy in bifunctional catalysts for selective conversion of hydrocarbons, *Nature,* 245–248 **(2015)** 528