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Structure Sensitivity in Catalysis by Sulfides

Henrik Topsøe
Haldor Topsøe Research Laboratories
Nymøllevej 55, DK-2800 Kgs. Lyngby, Denmark

Sulfide-based hydrotreating catalysts play an increasing role in the production of clean transport fuels. Some of the most refractory sulfur compounds, like 4,6 dimethyldibenzothiaphene, which need to be desulfurized react via two pathways, a so-called "direct" hydrogenolysis path and a "hydrogenation" path involving pre-hydrogenation of one of the aromatic rings. Although the existence of such pathways has been known for about 30 years, it has been difficult to get detailed insight into the nature of the active sites and most of the information about the structure sensitivity of reactions has come from kinetic investigations and structure-activity relationships. Recently, it has been possible by use of STM and DFT to gain direct insight into the nature of the reactions and the sites. This has provided a much better understanding of the origin of structure sensitivity in such catalysts. Moreover, the insight has facilitated to the introduction of more active and selective industrial catalysts.