Generation of Structurally Defined Sites on Surfaces: Towards Well-defined Heterogenous Catalysts

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Abstract:

Nearly all large-scale catalytic reactions in chemical industry use a heterogeneous catalyst. These critically important materials usually contain a high surface area inert support (SiO_2, Al_2O_3, etc.), and a catalytically active site dispersed on the support. The structure of an active site in a heterogeneous catalysts can be extremely difficult to determine using spectroscopic techniques because available synthetic methods produce complex mixtures of active and dormant sites on a support surface. This limitation results in empirical optimization strategies, and also reactions that are less energy efficient than those catalyzed by related homogeneous catalysts. This seminar will describe our efforts to generate well-defined active site structures on oxide surfaces, and applications of these strategies to study a model industrial catalyst. Generation of very strong Lewis acid sites on surfaces, such as well-defined silylium (R_3Si^+) sites on oxides, will be discussed and related to how substrates interact with surfaces. These studies relate to support effects common in heterogeneous olefin polymerization catalysts, which will be described in the context of a model heterogeneous olefin polymerization catalyst containing an oxide, alkylaluminium, and a zirconocene precatalyst used in industrial polyethylene synthesis.