Determination of Active Sites for Oligomerization in Heterogeneous Catalysts with Nitrogenous Compounds as Probe Molecules

F. Nadolny*, S. Peitz*; R. Franke*, W. Reschetilowski**
*Evonik Performance Materials GmbH, Marl, Germany, **TU Dresden,Germany

Abstract

C-C bond formation is the basis of the chemical industry to produce complex molecules from C_2 to C_4 feedstocks. For example the *n*-butene containing fraction can be oligomerized to longer-chain compounds [1] which are usually used as precursors for the production of PVC plasticizers [2]. This reaction can be heterogeneously catalyzed under industry-like conditions on $NiO\text{-}Al_2O_3/SiO_2$ catalysts. The presence of aluminum plays a crucial role in the formation of active nickel sites [1]. If there is no interaction between nickel and surface aluminum atoms, remaining acid sites can affect the product distribution towards undesired products [3]. Both, acid and nickel sites catalyze the C-C bond formation by interaction with the electron rich double bond of the olefins. By using probe molecules with the same size compared to the reactant the accessible active sites of the catalyst can be measured. Furthermore, it is possible to distinguish between LEWIS and BRØNSTED acid sites by means of suitable spectroscopic methods. Various alkylamines and pyridine derivates were adsorbed on an amorphous aluminosilicate. The interaction between amine and the aluminosilicate was analyzed by XPS and ^{27}Al MAS NMR spectroscopy. Depending on the steric properties of the pyridine derivates, acid sites with a specific surface structure can be selectively masked.

The preferred precursors for the formation of catalytically active coordination sites can be determined by *in situ* impregnation of the amine-modified aluminosilicates with a nickel-containing solution. The results indicate that the presence of LEWIS acid sites plays a key role in the formation of active nickel sites.

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