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# Applications of XAS in Heterogeneous Catalysis Research

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X-ray absorption spectroscopy (XAS) has many uses in heterogeneous catalysis research, and its main applications will be described. X-rays are an ideal probe for catalyst samples because they generally do not induce reactions in sample materials or perturb their physical state. They are also able to penetrate sample cell walls and can be used at high pressure and temperature making them ideal for in situ studies. One of the simplest applications of XAS, both in the form of extended fine structure (EXAFS) spectroscopy and near-edge structure (XANES) spectroscopy, is to provide information about the spatial and electronic structure of highly dispersed catalytic species. When the species are in the form of clusters of size less than 4 nm, they cannot be observed by conventional structural tools like x-ray diffraction, but can be readily identified with XAS. An example of this application will be given for supported manganese oxide catalysts for oxidation reactions, where a shift in rate-determining step can give rise to a change in coordination. One of the limitations of XAS is that it is difficult to apply with liquids because, although solvents like water or hydrocarbons do not interfere chemically with x-rays, they do absorb them and attenuate beam intensity. For this reason most heterogeneous catalysis studies have been carried out in the gas-phase. However, special cells with chemically and thermally tolerant windows allow the use of in situ conditions. A recent example of a study of nickel phosphide catalysts for hydrodesulfurization carried out in the liquid-phase at reaction conditions will be described where XAS studies allow identification of the active site, and its state during reaction. A recent unique application of XAS for the measurement of reaction rates will also be described. This is carried out by transient measurements of coverage, and is used to show that hydroperoxide species are reactive intermediates in the epoxidation of propylene in titanosilicate-supported gold catalysts.