

Pd nanoparticles solid-liquid interface study during liquid phase selective hydrogenation by combined XAS and ATR-IR

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Hydrogenation reactions occupy an important place in the realm of catalysis with various functional groups such as double and triple bonds and aldehydes among others which can undergo hydrogenation to produce diverse intermediates and fine chemicals [1]. In the fine chemical industry, these reactions are often performed in liquid phase due to the thermal stability and sensitivity of the compounds. Hydrogenation of furfural in liquid phase was chosen as a model hydrogenation reaction because the conversion and product selectivity are sensitive to both temperature of reaction and solvent [2]. Our aim is to understand the composition of the solid-liquid interface and how solvents and reaction conditions influence on the conversion and the product selectivity of a specific metal. For this purpose, we used X-ray absorption spectroscopy (XAS) to monitor the oxidation state and local environment of Pd during reduction and reaction in the liquid phase (5 bar). Infrared spectroscopy in the attenuated total reflectance mode (ATR-IR) was exploited to follow the nature of the adsorbed species under similar reaction conditions. A commercial reduced 5 wt.% Pd/Al₂O₃ was used to perform hydrogenation of furfural in three solvents (isopropanol, cyclohexane and toluene). The Pd nanoparticles were partially oxidized by storage in air but were fully reduced at 125°C before changing to the hydrogenation reaction conditions. During reduction, the XANES features of Pd metal shifted to lower energy, which together with the increase of the Pd-Pd bond distance from 2.74 Å to 2.81 Å are signatures of the formation of hydrides on the Pd surface. Admittance of the hydrogenation mixture containing furfural consumed these species. The intensity of the XANES features and the Pd-Pd bond distance after reduction of Pd were different depending on the solvent suggesting that the hydrogen coverage is governed by the selected solvent. ATR-IR spectroscopy allowed monitoring the adsorption and reaction of furfural at the surface of the catalyst when admitting the furfural solution to the catalyst after reduction. The observation of adsorbed CO on Pd metal was related to the formation of furan, which is the major product of furfural decarbonylation in cyclohexane and isopropanol. Lower CO signals together with the absence of a-top CO were observed in toluene, in which solvent, furfuryl alcohol is the major product, indicating that hydrogenation of furfural is taking place on specific sites.

References

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