The Effect of Surface Basicity Modification on H_2 Adsorption Properties over Au/TiO_2 Catalysts

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Abstract: The global hydrogen production of the chemical industry exceeds 50 million tons annually, which is used for several important industrial processes. However, because hydrogen molecules have low reactivity owing to their strong and non-polar bond as well as low polarizability, they can only be activated directly with a limited range of chemical systems under mild conditions. Thus, understanding hydrogen activation properties in catalytic systems can contribute to the development of more efficient approaches in H_2-based processes of interest. Also, among the various catalysts, Au catalysts have been investigated for a variety of reactions, including CO preferential oxidations, semi-hydrogenation, and organic oxidations. Especially, in the hydrogenation industry, Au catalysts are attractive alternatives to Pd-, Pt-, and Ni-based catalysts due to the high intrinsic alkene selectivity of Au. Over the past decades, palladium, platinum, and nickel have been widely used by the alkyne partial hydrogenation industry, but these metals have low intrinsic alkene selectivity owing to the over hydrogenation to alkane and oligomerization reactions. However, even though Au catalysts have considerable selectivity, they have a well-known low hydrogenation activity, which is orders of magnitude lower than other metal catalysts. Thus, if the fundamental chemistry of hydrogen activation and low hydrogen coverage can be understood and improved, this can offer numerous opportunities to consider new catalysts and catalytic processes for selective hydrogenation. In this work, therefore, we modified the surface basicity of Au/TiO_2 to improve hydrogen adsorption properties. The key parameters for H_2 activation are the hydrogen adsorption capacity, the strength of hydrogen adsorption, and hydrogen atom equivalent transport through the support. We analyzed the changes of surface chemistries and H_2 adsorption properties with TGA, titration, FT-IR, and volumetric chemisorption.