

Structure–Activity Relationship for Dehydrogenative H₂ Release from
N-Containing Liquid Organic Hydrogen Carrier using Pd-Supported Metal Oxide Catalysts

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To make the hydrogen economy feasible, it is necessary to develop technologies that safely store and transport hydrogen. Liquid organic hydrogen carrier (LOHC) technology is considered as one of the promising means for this purpose. Recently, perhydro-2-(n-methylbenzyl)pyridine (H₁₂-MBP) with H₂ storage density of 6.15 wt% has been designed and synthesized in the laboratory. In this study, we investigated the effect of the metal oxides supporting Pd catalysts on their catalytic performances during H₂ release from H₁₂-MBP via dehydrogenation. Various types of Pd supported metal oxides (Al₂O₃, CeO₂, TiO₂, ZrO₂, SnO₂) were synthesized and their catalytic activities were correlated with the surface characteristics of the metal oxides such as acidity, adsorption affinity, and charge transfer value of H₁₂-MBP, which determined via combined experimental and theoretical studies. Of all tested metal oxides, Pd supported Al₂O₃ presented the largest H₂ yield and the highest dehydrogenation rate. Pd supported CeO₂ was the most stable and exhibited reasonably high catalytic activity with the best recyclability and this was attributed to the strong metal–support interaction.