

Hydrogen Activation by Transition Metals

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Supported transition metal clusters and small particles act as catalysts for the hydrogenation and dehydrogenation of hydrocarbons. Using density functional calculations on models of simple and embedded clusters models, we discuss the structural and energetic consequences of hydrogen loading of zeolite supported small transition metal clusters of definite nuclearity, in particular for the cases of Rh₆ and Ir₄ [1–3]. Silver, a widely used oxidation catalyst, was recently shown to catalyze the regioselective hydrogenation of unsaturated aldehydes to unsaturated alcohols. We discuss the activation of molecular hydrogen by silver and the hydrogenation reaction using a slab model density functional approach [3,4].

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