

C-H bond activation by solid oxides – mechanisms and catalysts

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Density functional theory (DFT) ‘in concert’ with experiments is used to examine the mechanisms of the oxidative dehydrogenation of alkanes (propane) and of alcohols (methanol) on supported transition metal oxides. Hydrogen abstraction by metal-oxo bonds is identified as rate-determining step.^{1,2} Theory helps to bridge the gap between powder catalysts and model systems consisting of oxide particles on thin films under surface science conditions.³ For vanadia catalysts different supporting oxides are compared. The special support effect of CeO₂ is found to be due to its unique ability to stabilize the highest oxidation state of vanadium.⁴ For vanadia on CeO₂ the dependence of the activity on the particle size is discussed.^{5,6}

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