Chromium Oxides Supported on Transition-Aluminas for Catalytic Dehydrogenation of Propane

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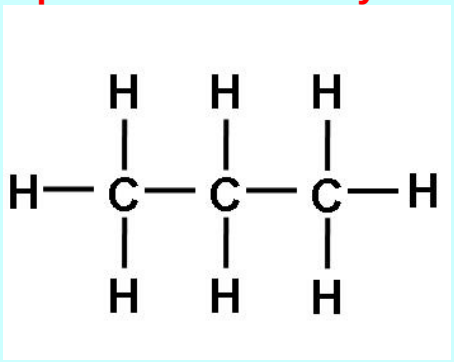
Chromium/transition-aluminas are well-known catalysts in petrochemical industry for the production of alkenes via dehydrogenation of alkanes. However, the atomic-scale mechanism of the role of Cr/transition-aluminas in the catalytic reactions still remains open.

First-principles quantum mechanical calculations for the catalytic chemical reaction of the dehydrogenation of a selected alkane, propane (C_3H_8), with the presence of Cr supported on γ-alumina (γ-Al_2O_3) have revealed that the dispersed chromium oxide species (CrO_3 and CrO_4) with the active oxygen sites play a key role in the dissociation of alkanes.

Propane - saturated hydrocarbon

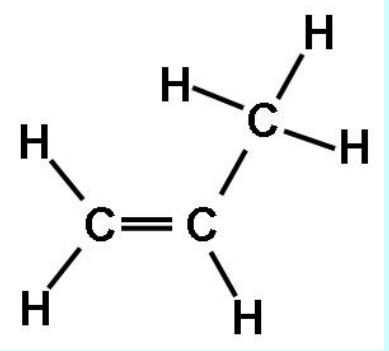


Dehydrogenation of alkanes

($C_nH_{2n+2} \rightarrow C_nH_{2n} + 2H$)

Catalytic CrO_x/transition-aluminas

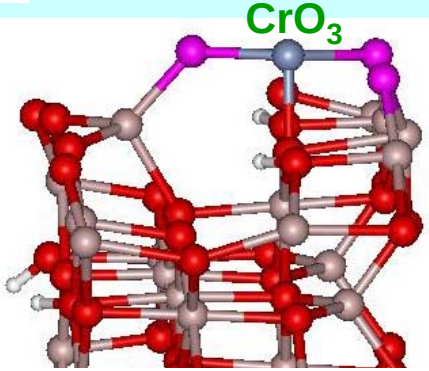
Propene - unsaturated hydrocarbon

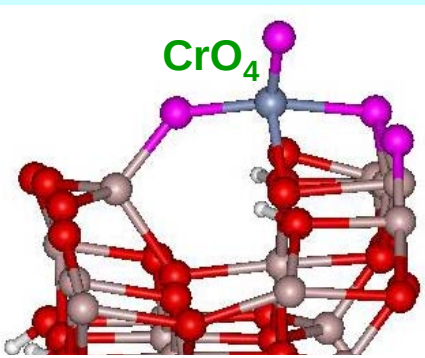


+ 2H

CrO_3 and CrO_4 supported on alumina act as catalysts.

All of the oxygen sites are active in trapping the hydrogen atoms.





Cr does not trap any hydrogen atoms, but it acts as the binding center that holds the active oxygen atoms.